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Simplified Multicomponent Fractionation Calculations.

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SIMPLIFIED MULTI-COMPONENT FRACTIONATION CALCULATIONS

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by
Raymond V. Bailey
B.S., Louisiana Polytechnic Institute, 1944
M.S., Louisiana State University, 1948
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ABSTRACT

In Chapter I several methods are presented for the calculation of minimum reflux ratio and the number of trays required in multi-component fractionation. These methods are presented as an improvement over certain previously published methods, in that the time required for calculations has been considerably shortened and the accuracy has been improved in many cases.

Part I contains a modification of the Scheibel-Montross (17) equation for minimum reflux. The temperatures are properly defined for systems in which the relative volatility varies. This modification places the calculation on a trial and error basis, but changes the reliability of the method from a maximum error of about fifteen percent to about one percent. The accuracy is about the same as the Colburn (3) correlation, but the time required in application is much less.

In Part II a pseudo reflux ratio and an equilibrium curve are defined in a more accurate manner for the application of the Scheibel (15) method for tray determinations. The modified method has a maximum error of about five percent compared to about twenty percent for the unmodified method.

Part III contains a graphical solution for tray requirements which is more advantageous than the modified Scheibel method of Part II if a heat balance around the feed point is necessary and the

minimum reflux ratio is not of primary significance. In addition, the proposed method permits a check on the assumed distribution of a split key.

The graphical solution presented is somewhat similar to the method proposed by Hengstebeck (8), but with the pseudo operating lines and equilibrium curve defined in such a manner as to permit application of the method at reflux ratios near the minimum as well as reflux ratios which are large compared to the minimum.

Multi-component systems are placed on the basis of the key components by the definitions:

$$x = \frac{X_{lK}}{\Sigma X_{keys}}$$

$$y = \frac{Y_{lK}}{\Sigma Y_{keys}}$$

The equilibrium curve and pseudo operating lines are determined by a calculation of the composition on the feed tray and the tray above the feed.

The proposed method requires fewer calculations than the method of Jenny (10) and eliminates the trial and error in the determination of the feed tray temperature.

The maximum error is about five percent.

Chapter II contains a modified solution of the equations involved in the Colburn (2) correlation for minimum reflux ratio which permits these relations to be satisfied with a considerable saving of time over that usually required. The time requirement for calculation compares favorably in all cases with the modified Scheibel-Montross (4) method as presented in Chapter I. In many cases the time requirement is reduced considerably, especially when the minimum reflux ratio is desired for several feed conditions for a given separation.

In Chapter III the application of Underwood's (7,8,9) equations and the Colburn (2) correlation for minimum reflux for the determination of the distribution of split keys at minimum reflux is presented. Equations have been developed to systematize the calculations and minimize the trial and error involved in the application of the Colburn correlation and Underwood's equations.

A study has been made of the distribution of split keys which will give the optimum number of trays at reflux ratios other than total and minimum. The distribution of split keys obtained at total reflux was found to give a minimum number of trays at all reflux ratios except those very close to the minimum. At this point the optimum distribution approaches that obtained at minimum reflux.

CHAPTER I

Simplified Multi-Component Fractionation Calculations

by
RAYMOND V. BAILEY
and
JESSE COATES

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Simplified Multi-Component Fractionation Calculations

Part I

MINIMUM REFLUX RATIO

RAYMOND V. BAILEY* and JESSE COATES**

THERE exist in the literature several methods of determining the minimum reflux ratio for a multi-component system.

The rigorous method, as defined by Jenny[11] involves tedious trial and error.

Underwood[18] developed equations for the exact determination of the minimum reflux for a multi-component system based on constant volatility and complete separation. However, for most actual cases, in which the volatility is not constant, the result is only a rough approximation.

Gilliland[7] presented an equation, based on equal ratio of the keys in the two pinches, which involves trial and error if the feed condition is other than a liquid at feed tray temperature. This equation gives a limiting low value. Later Robinson and Gilliland[14] developed an equation which gave a limiting high value. The recommended procedure is to take the average of the limiting values for the true minimum reflux ratio. However, the limits are often so far apart as to leave the true minimum reflux ratio in doubt.

Colburn[3] pointed out that the ratio of the keys in the pinches at minimum reflux ratio are not equal and developed an empirical expression for the relation of the keys at minimum reflux. The relation has an accuracy of approximately one percent, but involves considerable trial and error.

Other methods[2,9] have been presented, based on the false assumption that the ratio of the keys in the pinches are equal at minimum reflux.

Scheibel and Montross[17] developed an empirical equation consisting of three terms:

1. The reflux to separate the key components, assuming that the components lighter than light key have infinite volatility and the components heavier than the heavy key have zero volatility.
2. The reflux to separate the heavier components from the overhead due to their actual volatilities.
3. The reflux to separate the lighter components from the bottoms due to their actual volatilities.

This equation is accurate within approximately one percent for systems in which the relative volatilities are constant. However, the equation needs slight modification and the temperatures must be properly defined for the cases in which the relative volatilities are not constant.

The essential equations presented by Scheibel and Montross[17] follow:

1. Pseudo ratio of liquid to vapor

$$m = \frac{M_L - \Sigma M_{hF}}{M_V - \Sigma M_{lF}} \qquad (1)$$

where

m = pseudo ratio of liquid to vapor
M_L = mols of liquid feed
M_V = mols of vapor feed
ΣM_{hF} = total mols of components heavier than the heavy key in the feed
ΣM_{lF} = total mols of components lighter than the light key in the feed

2. Definition of McCabe-Thiele type diagram on the basis of two key components as follows:

$$x = \frac{X_{lK}}{X_{lK} + X_{hK}} \qquad (2)$$

$$y = \frac{Y_{lK}}{Y_{lK} + Y_{hK}} \qquad (3)$$

where

IN THIS article several methods are presented for the calculation of minimum reflux ratio and the number of trays required in multi-component fractionation. These methods are presented as an improvement over certain previously published methods, in that the time required for calculations has been considerably shortened and the accuracy has been improved in many cases.

Part I contains a modification of the Scheibel—Montross[17] equation for minimum reflux. The temperatures are properly defined for systems in which the relative volatility varies. This modification places the calculation on a trial and error basis, but changes the reliability of the method from a maximum error of about 15 percent to about 1 percent. The accuracy is about the same as the Colburn[3] correlation, but the time required in application is much less.

In Part II (to appear in a later issue) a pseudo reflux ratio and an equilibrium curve are defined in a more accurate manner for the application of the Scheibel[17] method for tray determinations. The modified method has a maximum error of about 5 percent compared to about 20 percent for the unmodified method.

Part III (also to appear later) contains a graphical solution for tray requirements which is more advantageous than the modified Scheibel method of Part II if a heat balance around the feed point is necessary and the minimum reflux ratio is not of primary significance. In addition, the proposed method permits a check on the assumed distribution of a split key.

The graphical solution presented is somewhat similar to the method proposed by Hengstebeck[8], but with the pseudo operating lines and equilibrium curve defined in such a manner as to permit application of the method at reflux ratios near the minimum as well as reflux ratios which are large compared to the minimum.

Multi-component systems are placed on the basis of the key components by the definitions:

$$x = \frac{X_{lK}}{\Sigma X_{Keys}}$$

$$y = \frac{Y_{lK}}{\Sigma Y_{Keys}}$$

The equilibrium curve and pseudo operating lines are determined by a calculation of the composition on the feed tray and the tray above the feed.

The proposed method requires fewer calculations than the method of Jenny[10] and eliminates the trial and error in the determination of the feed tray temperature.

The maximum error is about 5 percent.

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x = equivalent liquid composition based on the key components only
y = equivalent vapor composition based on the key components only
X_{lK} = liquid composition of the light key
X_{hK} = liquid composition of the heavy key
Y_{lK} = vapor composition of the light key
Y_{hK} = vapor composition of the heavy key

3. Empirical equation for minimum reflux ratio

$$R_M = \frac{1}{M_{lKF} + \Sigma M_{lF}} \left[M_{lKF} R'_M + \frac{M_{hKF} + \Sigma M_{hF}}{M_F} \sum \frac{M_{hF}}{\frac{K_{lK}}{K_h} - 1} + \sum M_{lF} \left(\frac{1 + \frac{K_{lK}}{K_l}}{\frac{K_l}{K_{hK}}} \right) \right]$$

where

R'_M = pseudo minimum reflux ratio based on the key components, determined from the McCabe-Thiele[1] type diagram defined, using the pseudo ratio of liquid to vapor.
R_M = true minimum reflux ratio
M = mols
K = equilibrium constant Y/X

Subscripts:

F = feed
h = component heavier than the heavy key
l = component lighter than the light key
hK = heavy key component
lK = light key component

The pseudo minimum reflux ratio, R'_M, gives the mols of reflux per mole of the key components overhead, but is used in the equation by Scheibel and Montross[17] as if it were mols of reflux per mole of the light key in the feed. The two may be equal in many cases, but not in all cases. Similarly, the correction term for the heavy components,

$$\frac{1}{M_F} \sum \frac{M_{hF}}{\frac{K_{lK}}{K_h} - 1}$$

is reflux per mole of bottoms; therefore, the equation should read as follows:

$$R_M = \frac{1}{D} \left[M_{KD} R'_M + \frac{W}{M_F} \sum \frac{M_{hF}}{\frac{K_{lK}}{K_h} - 1} + \sum M_{lF} \left(\frac{1 + \frac{K_{lK}}{K_l}}{\frac{K_l}{K_{hK}}} \right) \right] \quad (4)$$

Where

D = total mols of overhead
M_{KD} = total mols of the key components overhead
W = total mols of bottoms

Temperatures for Pseudo Minimum Reflux

The purpose of the pseudo ratio of liquid to vapor is to correct the operating lines to a basis which will permit the use of the McCabe-Thiele type diagram defined. However, this pseudo ratio of liquid to vapor does not correct the equilibrium curve for the presence of the light components, whose relative volatility is assumed to be infinite, in the vapor and the heavy components, whose relative volatility is assumed to be zero, in the liquid of the fractionating and stripping sections respectively.

For the stripping section, if the relative volatilities of the heavy components are assumed to be zero

$$\Sigma X_{Keys} = 1 - \frac{\Sigma M_{hF}}{L_m}$$

and for the fractionating section, assuming the light components to have infinite volatility

$$\Sigma Y_{Keys} = 1 - \frac{\Sigma M_{lF}}{V_n}$$

where

L_m = liquid downflow in the stripping section
V_n = vapor upflow in the fractionating section

Thus, the temperatures of the pinches will correspond to the reflux ratio of $\frac{M_{KD} R'_M}{D}$ with the light components in the vapor phase of the fractionating pinch and the heavy components present in the liquid of the stripping pinch.

These temperatures may be determined by rearrangement of the operating lines. Thus,

For the fractionating section pinch:

$$K_{hK} = \frac{L_n}{V_n} + \frac{D X_D}{V_n X_{hkn}}$$

NOMENCLATURE

α = Relative volatility with respect to heavy key
d = Mols of component in overhead
D = Total mols overhead
f = Function
K = Equilibrium constant = Y/X
l = Mols of component in liquid phase
L = Mols of liquid downflow in column
m = Pseudo ratio of liquid to vapor
M = Mols of component
N = Number of theoretical trays
R = Reflux ratio, mols reflux per mole of overhead
R' = Pseudo reflux ratio, mols reflux per mole of keys overhead
v = Mols of component in vapor phase
V = Mols of vapor upflow in tower
w = Mols of component in bottoms
W = Total mols of bottoms
x = Mol fraction of light key in liquid on two-component basis.
X = Mol fraction of component in liquid phase
y = Mol fraction of light key in vapor on two-component basis.
Y = Mol fraction of component in vapor phase
z = Mol fraction of light key in vapor plus liquid on two-component basis
Z = Total mol fraction of component (liquid + vapor)

Subscripts:

D = Overhead
f = Feed tray
F = feed
h = heavy component, heavier than heavy key
hK = heavy key
i = intersection of operating lines
l = light component, lighter than light key
lK = light key
L = liquid
m = stripping section
M = minimum
n = fractionating section
t = top tray
v = vapor
w = bottoms

Superscripts:

$'$ = pseudo

and for the stripping section pinch:

$$K_{lK} = \frac{L_m}{V_m} + \frac{W X_w}{V_n X_{lKm}}$$

where $\frac{L_n}{V_n}$ and $\frac{L_m}{V_m}$ are calculated using the reflux ratio $\frac{M_{KD} R'_M}{D}$.

where

K_{hK} = equilibrium constant for heavy key component
K_{lK} = equilibrium constant for light key component
X = mole fraction in liquid phase
L = mols liquid
V = mols vapor

Subscripts:

hKn = heavy key in fractionating pinch
lKm = light key in stripping pinch
D = overhead
W = bottoms
m = stripping section
n = fractionating section

The equilibrium curve may be broken at a point between the stripping section and the fractionating section. At the pseudo minimum reflux ratio the operating lines will cross their respective equilibrium curves at the same value of "x" and intersect on the pseudo feed line between the two sections of the equilibrium curve.

The temperature for the separation of the heavier components is the temperature of the stripping column pinch at the true minimum reflux ratio, since that temperature determines the concentration of the components in the pinch and therefore the minimum reflux ratio.

Similarly, the temperature for separation of the lighter components has significance only in the fractionating pinch corresponding to the true minimum reflux ratio.

However, the correction terms are usually small and/or the variation of the relative volatility between the pinch temperatures is not great, and usually only slight error is introduced by using the "K" values at the temperatures of the pinches corresponding to the reflux ratio $\frac{M_{KD} R'_M}{D}$. If the correction factors and the variation of the relative volatility of the components are large, recourse to trial and error is necessary.

Recommended Methods of Determination of R'_M

METHOD I:

As a very close approximation, the operating lines intersect the pseudo feed line at a relative volatility of the key components which is the average of the relative volatilities of the pinches corresponding to the reflux ratio $\frac{M_{KD} R'_M}{D}$.

The equation of the pseudo feed line is given by

$$y = z_F + m(z_F - x)$$

and from the simulation of the fractionating pseudo operating line with this pseudo feed line at the pinch, eliminating *y*:

$$x_i = \frac{z_F (1 + m) - \frac{x_D}{R'_m + 1}}{\left(\frac{L_n}{V_n}\right)' + m} \qquad (5)$$

where

x_i = liquid composition on basis of the key components at the intersection of the pseudo operating line and the pseudo feed line.
z_F = mole fraction of light key in the feed on basis of the key components.
m = pseudo ratio of liquid to vapor.
x_D = mole fraction of light key in overhead on basis of key components.
R'_M = pseudo minimum reflux ratio.
$\left(\frac{L_n}{V_n}\right)'$ = pseudo ratio of liquid to vapor in fractionating section.

If m equals infinity, then $x_i = z_F$.

From Fenske[4] equation for binary mixtures:

$$R'_M = \frac{1}{\alpha_{avg} - 1}\left[\frac{x_D}{x_i} - \alpha_{avg}\left(\frac{1 - x_D}{1 - x_i}\right)\right] \qquad (6)$$

where

$$\alpha_{avg} = \frac{\alpha_n + \alpha_m}{2}$$

α_n = relative volatility of the key components at the fractionating pinch corresponding to a reflux ratio

$$\frac{M_{KD} R'_M}{D}$$

α_m = relative volatility of keys at the stripping pinch corresponding to a reflux ratio of

$$\frac{M_{KD} R'_M}{D}$$

The relative volatilities at the pinches may be determined by noting that a rearrangement of the operating lines at the pinches gives:

For fractionating section

$$K_{hK} = \frac{L_n}{V_n} \text{ Approx.} \qquad (7)$$

For stripping section

$$K_{lK} = \frac{L_m}{V_m} \text{ Approx.} \qquad (8)$$

To calculate R'_M:

1) Assume a value of R'_M;
2) Calculate x_i by equation 5;
3) Calculate the average relative volatility;
4) Calculate R'_M by equation 6;
5) Use calculated value of R'_M for second assumption and repeat until assumed R'_M equals calculated R'_M.

Usually the second trial is sufficient since the convergence is very rapid.

It must be emphasized that this method is only approximate and therefore should be used only to obtain a first assumption for Method II if the separation is extremely poor or if the relative volatility of the keys is below 1.5 with a large spread between the pinches.

METHOD II:

The pinch compositions are calculated assuming the light components have infinite volatility and the heavy components have zero volatility. Trial and error is used until the ratio of the liquid concentrations of the key components in the two pinches are equal, which must be the case for a binary system.

The operating lines, at the pinches, may be written in the following form:

$$X_n = \frac{X_D}{K + (K - 1)\frac{L_n}{D}} \qquad (9)$$

$$X_m = \frac{X_w}{K + (1 - K)\frac{L_m}{W}} \qquad (10)$$

where

X_n = concentration of a component in the fractionating pinch
X_m = concentration of a component in the stripping pinch
K = equilibrium constant of component in question
L_n/D = ratio of moles of liquid in fractionating section to moles of overhead
L_m/W = ratio of moles of liquid in stripping section to moles of bottoms
X_D = mole fraction of component in question in overhead
X_w = mole fraction of component in question in bottoms

At the pinches, since the light components have infinite volatility and the heavy components are considered to have zero volatility

$$\Sigma X_n = O \text{ for the light components} \quad (11)$$

$$\Sigma Y_n = \frac{\Sigma M_{1F}}{V_n} \text{ for the light components} \quad (12)$$

$$\Sigma X_m = \frac{\Sigma M_{hF}}{L_m} \text{ for the heavy components} \quad (13)$$

$$\Sigma Y_m = O \text{ for the heavy components} \quad (14)$$

and for this case, at a reflux ratio of $\frac{M_{KD} R'_M}{D}$

$$\frac{r_m}{r_n} = 1.00 \quad (15)$$

where

r_m = ratio of the key components in the liquid phase at the stripping pinch
r_n = ratio of the key components in the liquid phase at the fractionating pinch

For purposes of illustration the debutanizer example of Scheibel[16] will be used

Sample Calculation

EXAMPLE 1

	Mols Feed	Mols Overhead	Mols Bottoms
C^3	1.0	1.0	
C^4	40.0	39.4	0.6
C^5	23.0	.4	22.6
C^6	16.0	....	16.0
C^7	12.0	....	12.0
C^8	8.0	....	8.0
		40.8	59.2

Feed at 220° F.
Mols Liquid 75.0
Mols Vapor 25.0
Operating pressure ..... 100 psia
Equilibrium constants are from the Nomograph in the same article [16].

Determination of R'_M

METHOD I:

Assume $\frac{M_{KD} R'_M}{D} = 1.4$

then $R'_M = \frac{1.4D}{M_{KD}} = \frac{(1.4)\ (40.8)}{39.8} = 1.435$

from equation (7)

$K_{c5} = \frac{(1.4)\ (40.8)}{(2.4)\ (40.8)} = 0.583$ approx. in fract. pinch

$K_{c4} = 1.38$ at the temperature at which $K_{c5} = 0.583$

This allows relative volatility at the upper pinch to be calculated.

From equation (8)

$$K_{c4} = \frac{(1.4)\ (40.8) + 75}{(2.4)\ (40.8) - 25} = \frac{L_m}{V_m}$$

$= 1.811$ approximate in stripping pinch

$K_{c5} = 0.82$ when $K_{c4} = 1.811$

$$\alpha_n = \frac{1.38}{0.583} = 2.365$$

$$\alpha_m = \frac{1.811}{0.82} = 2.21$$

$$\alpha_{avg} = 2.288$$

From equation (1)

$$m = \frac{M_L - \Sigma M_{hF}}{M_V - \Sigma M_{1F}} = \frac{75 - 36}{25 - 1} = 1.622$$

$$x_D = \frac{39.4}{39.4 + 0.4} = 0.99$$

$$z_F = \frac{40}{40 + 23} = .635$$

Using equation (5)

$$x_1 = \frac{(0.635)\ (2.622) - \frac{.99}{2.435}}{\frac{1.435}{2.435} + 1.622} = .572$$

From equation (6)

$$R'_M = \frac{1}{1.288}\left[\frac{.99}{.572} - 2.288\left(\frac{.01}{.428}\right)\right] = 1.30 \text{ first approximation}$$

Assume $R'_M = 1.30$

Then $\frac{(M_{KD})\ (1.30)}{D} = \frac{(39.8)\ (1.30)}{40.8} = 1.27$

Fractionating pinch:

$$K_{c5} = \frac{1.27}{2.27} = .56 \ ; \ K_{c4} = 1.33$$

Stripping pinch:

$$K_{c4} = \frac{(1.27)\ (40.8) + 75}{(2.27)\ (40.8) - 25} = 1.87 \ ; \ K_{c5} = .85$$

$\alpha_n = 2.375$
$\alpha_m = 2.200$
$\alpha_{avg} = 2.287$

$$x_1 = \frac{(.635)\ (2.622) - \frac{.99}{2.3}}{\frac{1.3}{2.3} + 1.622} = .570$$

$$R'_M = \frac{1}{1.287}\left[\frac{.99}{.57} - 2.287\left(\frac{.01}{.43}\right)\right] = \underline{1.31}$$

$$\frac{M_{KD} R'_M}{D} = \frac{(39.8)\ (1.31)}{40.8} = \underline{1.28}$$

METHOD II:

As a first assumption:

$$\frac{M_{KD} R'_M}{D} = 1.28 \text{ from } \textbf{Method I.}$$

$\frac{L_n}{V_n} = \frac{1.28}{2.28} = .561$ = Approximate K_{c5} at fractionating pinch

$V_n = (2.28)\ (40.8) = 93.0$
$L_m = (1.28)\ (40.8) + 75.0 = 127.2$

$\frac{L_m}{V_m} = \frac{127.2}{68} = 1.871$ = Approximate K_{c4} at stripping pinch

$\frac{L_m}{W} = \frac{127.2}{59.2} = 2.15$

Pinch temperatures are assumed using the approximate values calculated above. The key components are calculated at the pinches using equations (9) and

TABLE 1

Comparison of Minimum Reflux Ratios for Section I

Problem	Reference	FEED COMPOSITION X_l	X_{lk}	X_{hk}	X_h	α_l	α_h	MINIMUM REFLUX RATIO Present Method	Colburn	Schiebel-Montross
1	....	....	.30	.30	.40	....	0.5	4.54	4.51	3.95
2	....	....	.30	.30	.40	....	0.8	5.12	5.13	4.47
3	....	.40	.30	.30	....	2.1	....	1.45	1.45	1.64
4	(15)	Dubutanizer illustrated						1.38	1.38	1.27
5	(10)	Depropanizer example of Jenny's						.95	.96	.95*

For Problems 1, 2 and 3 the K values for the keys are given in Figure 1. Only a trace of the heavy key goes overhead and a trace of the light key in in the bottoms. Feed is liquid at the boiling point.

* Schiebel-Montross has compensating errors.

(10). The light and heavy components are determined from equations (11) through (14). The assumed temperatures are checked by a boiling point determination. The results are summarized below in tabular form.

Fractionating pinch:

	K_{174}	X_n	Y_n
C_3	3.29	-	.011
C_4	1.33	.551	.735
C_6	.56	*.449	.251
		1.000	.997

* by difference

Stripping pinch:

	K_{211}	X_m	Y_m	K_{210}	X_m	Y_m
C_4	1.87	*.393	.735	1.85	*.396	.732
C_5	.85	.325	.276	.84	.322	.270
C_6	-	-	-	.40	-	-
C_7	-	.282	-	.188	.282	-
C_8	-	-	-	.092	-	-
		1.000	1.011		1.000	1.002

* by difference

$$r_m = \frac{\frac{.396}{.322}}{\frac{.551}{.449}} = 1.00$$

Therefore $\frac{M_{KD} R'_M}{D} = \underline{\underline{1.28}}$

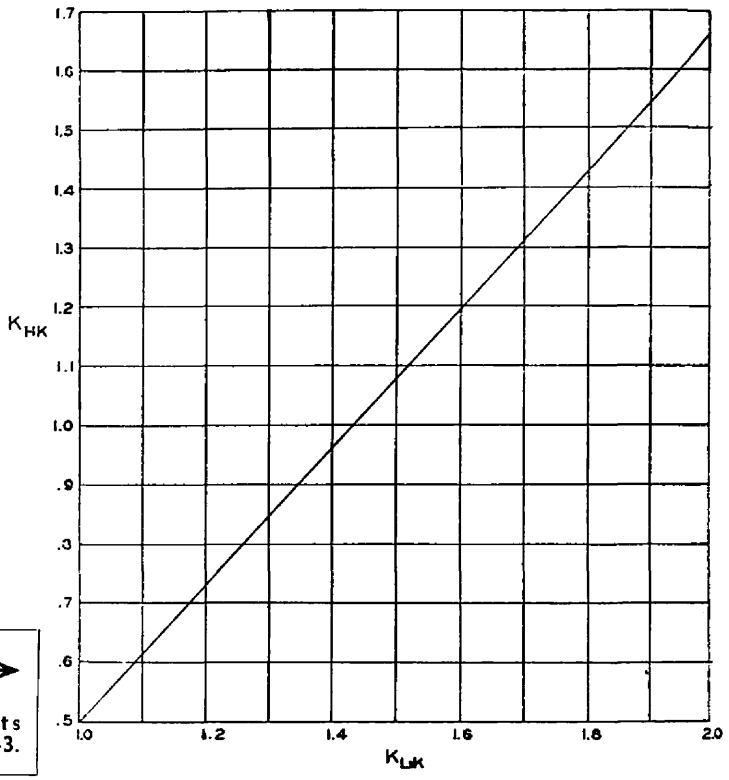

FIGURE 1
Equilibrium Constants for Keys—Problems 1-3.

From equation (4)

$$R_M = 1.28 + \frac{59.2}{40.8}\left[\frac{.16}{\frac{1.86}{.40}-1} + \frac{.12}{\frac{1.86}{.188}-1} + \frac{.08}{\frac{1.86}{.092}-1}\right] + \frac{1.0}{40.8}\left[\frac{1+\frac{1.35}{3.29}}{\frac{3.29}{.565}}\right]$$

$$R_M = 1.28 + 0.89 + .006 = \underline{\underline{1.38}}$$

It may be noted that the "K" values for the correction terms were taken at the pinch temperatures corresponding to a value $\frac{M_{KD} R'_M}{D} = 1.28$ rather than the true minimum reflux ratio 1.38. However, it should again be emphasized that, had the correction term been large compared to $\frac{M_{KD} R'_M}{D}$, for precise results another calculation would have been necessary, using the first value of R_M (1.38) to determine the "K" values at the pinches.

Discussion and Conclusions

In Table 1 a few results of the present method are compared with results obtained by the Scheibel-Montross[17] and the Colburn[3] methods. The present method shows a maximum deviation of 1 percent from the Colburn[3] method, while that of Schiebel-Montross[17] shows a maximum deviation of 13 percent.

Since the correlation of Colburn[3] holds extremely well for systems of constant volatility and should be equally as reliable for systems in which the volatility varies, no stepwise calculations were made for comparison.

The method presented is as reliable as the correlation of Colburn[3] and requires considerably fewer calculations, especially as the number of components in the system becomes large.

Simplified Multi-Component Fractionation Calculations

Part II

MULTI-COMPONENT TRAY CALCULATIONS

RAYMOND V. BAILEY and JESSE COATES

IN THIS second installment of a three-part series, the authors continue with a presentation of calculation procedures applicable to multicomponent fractionation. In part I, which appeared in the January, 1948, issue of *Petroleum Refiner*, a modification of the Scheibel-Montross[17] equation for minimum reflux was treated.

In this section, Part II, a pseudo reflux ratio and an equilibrium curve are defined in a more accurate manner for the application of the Scheibel[15] method for tray determinations. The modified method has a maximum error of about 5 percent compared to about 20 percent for the unmodified method.

Part III (which will appear later) contains a graphical solution for tray requirements which is more advantageous than the modified Scheibel method of Part II if a heat balance around the feed point is necessary and the minimum reflux ratio is not of primary significance. In addition, the proposed method permits a check on the assumed distribution of a split key.

The graphical solution presented is somewhat similar to the method proposed by Hengstebeck[8], but with the pseudo operating lines and equilibrium curve defined in such a manner as to permit application of the method at reflux ratios near the minimum as well as reflux ratios which are large compared to the minimum.

Multi-component systems are placed on the basis of the key components by the definitions:

$$x = \frac{X_{1K}}{\Sigma X_{Keys}}$$

$$y = \frac{Y_{1K}}{\Sigma Y_{Keys}}$$

The equilibrium curve and pseudo operating lines are determined by a calculation of the composition on the feed tray and the tray above the feed.

The proposed method requires fewer calculations than the method of Jenny[20] and eliminates the trial and error in the determination of the feed tray temperature.

The maximum error is about 5 percent.

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THIS section contains a modification of Scheibel's[15] method of tray determination for a multi-component system. The pseudo reflux ratio and the equilibrium curve are properly defined so that the method is, in general, reliable within 5 percent.

The first rigorous method for multi-component tray calculations involved considerable trial and error in matching components at the feed tray. Jenny[11] described a method of calculating the feed tray composition, thus eliminating the trial and error in matching components. Robinson and Gilliland[14] proposed an "alpha" method which simplified the equilibrium calculations at each tray. However, even with these simplifications, the method is long and laborious.

Jenny[11] proposed a graphical solution for multi-component tray requirements which involved several tray calculations to determine the equilibrium curve for the keys. The accuracy of the method depends on a choice of the feed tray temperature and the number of tray calculations made to establish the equilibrium curve. For a system with several components the work becomes rather laborious.

Hummel[10] expanded the method of Jenny[11] and applied it to the case of components with volatilities intermediate between the keys.

Jenny and Cicalese[12] presented a method of plotting a multi-component system on a two-component diagram by combining all light components with the light key and all heavy components with the heavy

NOMENCLATURE

α = Relative volatility with respect to heavy key
d = Mols of component in overhead
D = Total mols overhead
f = Function
K = Equilibrium constant = Y/X
l = Mols of component in liquid phase
L = Mols of liquid downflow in column
m = Pseudo ratio of liquid to vapor
M = Mols of component
N = Number of theoretical trays
R = Reflux ratio, mols reflux per mole of overhead
R′ = Pseudo reflux ratio, mols reflux per mole of keys overhead
v = Mols of component in vapor phase
V = Mols of vapor upflow in tower
w = Mols of component in bottoms
W = Total mols of bottoms
x = Mol fraction of light key in liquid on two-component basis.
X = Mol fraction of component in liquid phase
y = Mol fraction of light key in vapor on two-component basis.
Y = Mol fraction of component in vapor phase
z = Mol fraction of light key in vapor plus liquid on two-component basis
Z = Total mol fraction of component (liquid + vapor)

Subscripts:

$_D$ = Overhead
$_f$ = Feed tray
$_F$ = feed
$_h$ = heavy component, heavier than heavy key
$_{hK}$ = heavy key
$_i$ = intersection of operating lines
$_l$ = light component, lighter than light key
$_{lK}$ = light key
$_L$ = liquid
$_m$ = stripping section
$_M$ = minimum
$_n$ = fractionating section
$_t$ = top tray
$_v$ = vapor
$_w$ = bottoms

Superscripts:

′ = pseudo

key. However, the method has the disadvantage of requiring one set of tray by tray calculations in order to determine the equilibrium curve.

Several correlations[2,7] have been presented for the estimation of trays at a given reflux ratio, based on the minimum reflux ratio and the trays at total reflux. These correlations are reliable within about ten percent.

Scheibel[15] introduced a graphical solution, but failed to properly define the pseudo reflux ratio and the equilibrium curve. Due to this, errors as great as 15-20 percent may be encountered on simple systems.

Scheibel's[15] method consists of plotting pseudo operating lines on a binary distillation curve of the key components and stepping off the trays as on the conventional McCabe-Thiele[1] diagram.

From the correlation

$$\frac{R-R_M}{R+x_i}=f\left(\frac{N-N_M}{N+1}\right)$$

the pseudo reflux is defined by Scheibel[15]

$$R'+x_i=(R+x_i)\frac{R'_M+x_i}{R_M+x_i}$$

where f = function
N = number of trays at given reflux ratio, R
N_M = number of trays at total reflux

The composition based on the keys and the pseudo feed line are the same as defined in Part I.

Modification of the Definition of the Equilibrium Curve

As pointed out in Part I, if the light components are considered to have infinite volatility and the heavy components are assumed to have zero volatility

For the stripping section

$$\Sigma X_{Keys}=1-\frac{\Sigma M_{hF}}{L'_m}$$

$$\Sigma Y_{Keys}=1.00$$

and for the fractionating section

$$\Sigma X_{Keys}=1.00$$

$$\Sigma Y_{Keys}=1-\frac{\Sigma M_{lF}}{V'_n}$$

Therefore the equilibrium curve may be defined for the stripping section

$$x=\frac{\left(\frac{1}{1-\frac{\Sigma M_{hF}}{L'_m}}\right)-K_{hK}}{K_{lK}-K_{hK}} \qquad (16)$$

$$y=\frac{K_{lK}}{K_{lK}-K_{hK}}\left[1-K_{hK}\left(1-\frac{\Sigma M_{RF}}{L'_m}\right)\right] \qquad (17)$$

and for the fractionating section

$$x=\frac{\left(1-\frac{\Sigma M_{lF}}{V'_n}\right)-K_{hK}}{K_{lK}-K_{hK}} \qquad (18)$$

$$y=\frac{K_{lK}\,x}{1-\frac{\Sigma M_{lF}}{V'_n}} \qquad (19)$$

These values of x and y may be used to construct the equilibrium curve.

Modified Definition of Pseudo Reflux Ratio

In order to equate

$$\frac{R-R_M}{R+x_i}=f\left(\frac{N-N_M}{N+1}\right)=\frac{R'-R'_M}{R'+x_i}$$

to solve for R', R and R_M must be converted to mols of reflux per mole of the key components overhead otherwise $R+x_i$ has no significance. Actually in the term $R+x_i$, the value of x_i should be slightly different from x_i in $R'+x_i$, but the difference in the result is, in general, negligible.

Therefore

$$\frac{\frac{D}{M_{KD}}(R-R_M)}{\frac{DR}{M_{KD}}+x_i}=\frac{R'-R'_M}{R'+x_i}$$

from which

$$R'+x_i=\left(\frac{DR}{M_{KD}}+x_i\right)\left(\frac{R'_M+x_i}{\frac{DR_M}{M_{KD}}+x_i}\right) \qquad (20)$$

Sample Tray Calculation for Part II

EXAMPLE II

The tray requirements for the debutanizer, illustrated in Example I, will be determined for a reflux ratio of 3.0 mols of reflux per mole of overhead.

EXAMPLE 1

	Mols Feed	Mols Overhead	Mols Bottoms
C_3	1.0	1.0	...
C_4	40.0	39.4	0.6
C_5	23.0	.4	22.6
C_6	16.0	....	16.0
C_7	12.0	....	12.0
C_8	8.0	....	8.0
	....	40.8	59.2

Feed at 220° F.
Mols Liquid..... 75.0
Mols Vapor..... 25.0
Operating pressure..... 100 psia.
Equilibrium constants are from the Nomograph in the same article [16].

From Example I, Part I:

$R'_M=1.31$
$R_M=1.38$
$x_i=0.57$
$m=1.622$
$R=3.00$

From equation (20)

$$R'+.57=\left(\frac{(40.8)\ (3.0)}{39.8}+.57\right)\left(\frac{1.31+.57}{\frac{(40.8)\ (1.38)}{39.8}+.57}\right)$$

$R'=2.85$
$L'_m=(2.85)\ (39.8)+75=188$ mols

For the stripping section:

$$\Sigma X_{Keys}=1-\frac{36}{188}=.808$$

From equations (16) and (17)

$$x=\frac{\frac{1}{.808}-K_{c5}}{K_{c4}-K_{c5}}=\frac{1.24-K_{c5}}{K_{c4}-K_{c5}}$$

$$y=\frac{K_{c4}}{K_{c4}-K_{c5}}\ (1-.808\ K_{c5})$$

K_{c4}	K_{c5}	x	y
2.31	1.15	.078	.139
2.21	1.10	.126	.221
2.09	1.00	.220	.368
1.92	0.90	.333	.515
1.77	0.80	.453	.645
1.67	0.75	.532	.715

For the fractionating section:

$$\Sigma Y_{Keys}=1-\frac{1}{(2.85+1)\ (39.8)}=.993$$

From Equations (18) and (19)

$$x=\frac{.993-K_{c5}}{K_{c4}-K_{c5}}$$

$$y=\frac{K_{c4}\,x}{.993}$$

K_{c4}	K_{c5}	x	y
1.40	0.60	0.491	0.692
1.23	0.50	0.675	0.836
1.04	0.40	0.926	0.970

$$x_D = \frac{39.4}{39.4 + 0.4} = 0.99$$

$$x_W = \frac{0.6}{0.6 + 22.6} = 0.026$$

$$z_F = \frac{40}{40 + 23} = 0.635$$

The equilibrium curves are plotted in Figure 2, along with the pseudo operating lines which intersect on the pseudo feed line. The trays are stepped off as on the conventional McCabe-Thiele[1] diagram.

Referring to Figure 2, it may be noted that the step at the intersection of the operating lines (the feed tray step) intersects both equilibrium curves. The intersection of this step with the stripping section curve represents the vapor concentration from the feed tray, while the intersection with the fractionating curve represents the vapor concentration above the feed point to the tray above the feed.

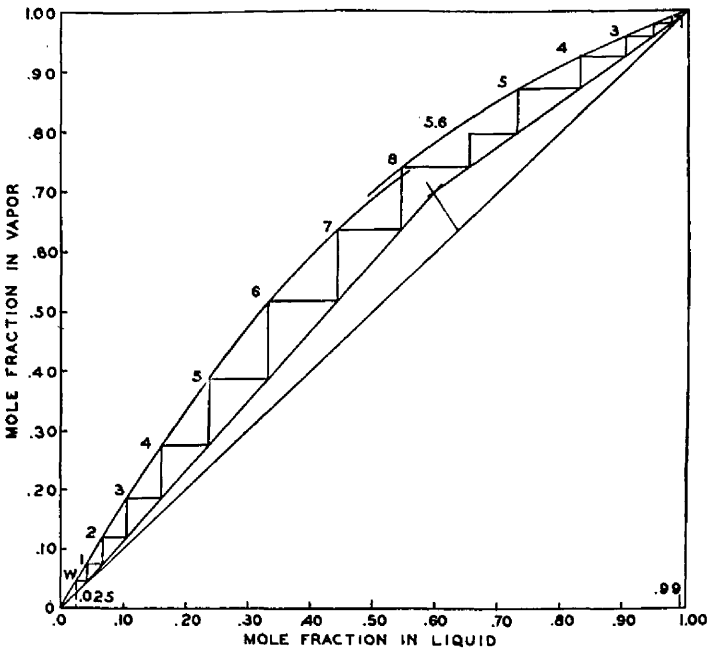

FIGURE 2

Determination of Trays for Example II

Discussion and Conclusions

Five illustrative examples have been selected from the literature and a comparison of the results by several methods has been made in Table 2. The maximum error by the present method was 3.5 percent, while Scheibel's[15] method gave a maximum error of 16 percent.

The accuracy of the method is limited by the reliability of the empirical correlation for obtaining the pseudo reflux ratio. However, in most cases the pseudo minimum reflux ratio approaches the actual minimum reflux ratio sufficiently close so that the correlation need hold only over a limited range. This makes the method, in general, more reliable than the correlations of Gilliland[7] and Brown and Martin.[2]

The present method has the further advantage of giving directly the optimum feed tray.

In preliminary design work, since, for many systems, the position of the equilibrium curve does not change appreciably for a moderate change in reflux ratio, one equilibrium curve calculation may suffice for the tray determinations at several reflux ratios.

TABLE 2A

Description of Illustrative Cases for Section II

Problem	Reference	FEED COMPOSITION X_l	X_{lk}	X_{hk}	X_h	RELATIVE VOLATILITIES α_l	α_{lk}	α_{hk}	α_h	PRODUCT COMPOSITION BASED ON KEYS Overhead	Bottoms
1	(14)	0.30	0.30	0.40	....	4	2	1	..	0.980	0.010
2	(14)	0.72	0.12	0.16	....	4	2	1	..	0.985	0.010
3	(14)	0.30	0.20	0.20	0.30	4	2	1	0.5	0.975	0.025
4	(15)	Debutanizer illustrated								0.99	0.026
5	(10)	Depropanizer example of Jenny's								0.988	0.023

TABLE 2B

Comparison of Tray Requirements for Section II

Problem	x_i	R_M	R'_M	R	R′ Author	R′ Scheibel	NO. OF THEORETICAL TRAYS STRIPPING Author	Calc.	Scheibel	FRACTIONATING Author	Calc.	Scheibel	Total Author	Calc.	Scheibel
1	0.500	1.127	1.88	3.00	5.12	4.40	8.5	8.9	8.5	7.1	7.3	7.5	15.6	16.2	16.0
2	0.726	0.500	1.25	0.74	2.03	1.68	11.1	10.7	11.0	8.8	8.8	9.4*	19.9	19.5	20.4*
3	0.610	0.913	1.47	1.78	3.03	2.66	8.1	7.3	8.6	6.7	7.0	7.1	14.8	14.3	15.7
4	0.57	1.38	1.32	3.00	2.85	2.80	8.0	8.0	6.2	5.6	5.6	5.5	13.6	13.6	11.7
5	0.47	0.95	2.05	1.50	3.26	3.03	9.0	Jenny 8.8	9.0	6.0	Jenny 5.7	8.3	15.0	Jenny 14.5	17.3

* Using Scheibel's figures, the author obtained 11 fractionating trays, total = 22.

Simplified Multi-Component Fractionation Calculations

Part III

MULTI-COMPONENT TRAY CALCULATIONS

RAYMOND V. BAILEY and JESSE COATES

OFTEN it is desirable, in order to make a heat balance around the feed tray, to know the feed tray composition and temperature as well as the tray requirements for a given reflux ratio. In many of these cases the true minimum reflux is not of primary significance. Therefore, it is desirable to have a rapid method of estimating the tray requirements without recourse to the calculaions necessitated in Parts I and II. (REFINER, January and February, 1948.)

Hengstebeck[8] placed multicomponent systems on a two-component basis by defining an equivalent ratio of liquid to vapor in each section of the column based on the pinch compositions. The definition of the equilibrium curve is correct only at total reflux, and the definition of the equivalent operating lines does not permit application of the method at reflux ratios approaching the minimum. In addition, heavy components or light components which might persist practically the entire length of the fractionating or stripping section, respectively, are not considered in the definition of the pseudo operating lines. Thus, in general, the method is applicable only to easily separated components at large reflux ratios.

Jenny's[11] method would suffice for the tray determinations, but the method offered here eliminates the trial and error in obtaining the feed tray temperature and the several multicomponent tray calculations required in order to establish the equilibrium curve for the Jenny[11] method.

In obtaining the feed tray composition and temperature, the feed tray action must be considered.

Gilliland[5] gives equations for the optimum feed tray for the following cases:

Case 1. Vapor entering the plate above the feed tray has the same composition as the vapor leaving the feed tray.

$$\left(\frac{X_{lK}}{X_{hK}}\right)_f \cong \left(\frac{X_{lK}}{X_{hK}}\right)_i \cong \left(\frac{X_{lK}}{X_{hK}}\right)_{f+1}$$

Case 2. Feed is part vapor. Vapor portion mixes physically with the vapor rising from the feed tray, but does not react with the feed tray liquid.

$$\left(\frac{X_{lK}}{X_{hK}}\right)_f \cong \left(\frac{X_{lK}}{X_{hK}}\right)_F \cong \left(\frac{X_{lK}}{X_{hK}}\right)_{f+1}$$

Case 3. Feed is all vapor and mixes with the feed tray vapor, but does not react with the liquid on the feed tray.

$$\left(\frac{X_{lK}}{X_{hK}}\right)_{f+1} \cong \left(\frac{X_{lK}}{X_{hK}}\right)_i \cong \left(\frac{X_{lK}}{X_{hK}}\right)_{f+2}$$

where

X_{lK} = Mole fraction of light key in liquid
X_{hK} = Mole fraction of heavy key in liquid

Subscripts:

f = feed tray
$f+1$ = tray above feed
$f+2$ = second tray above feed
i = intersection of operating lines of key components
F = feed

Since, as pointed out by Gilliland,[5] the optimum feed tray is a function of the feed tray action, multicomponent calculations will be placed on a two-component basis for both types of feed tray action.

In general, the feed tray action will have no appreciable effect on the total number of trays, but the optimum feed tray and feed tray temperature may be considerably affected.

Case I: The Feed Vapor Is Considered in Equilibrium with the Feed Tray Liquid

If the equivalent composition based on the key

THIS is the third and final part of a series which has appeared in consecutive issues of *Petroleum Refiner* presenting calculation procedures applicable to multi-component fractionation. In Part I a modification of the Scheibel-Montross[17] equation for minimum reflux was treated. In Part II a psuedo reflux ratio and an equilibrium curve was defined for the application of the Scheibel[15] method of tray determinations. This Part III contains a graphical solution for tray requirements which is more advantageous than the modified Scheibel method of Part II if a heat balance around the feed point is necessary and the minimum reflux ratio is not of primary significance. In addition, the proposed method permits a check on the assumed distribution of a split key.

The graphical solution presented is somewhat similar to the method proposed by Hengstebeck[8], but with the pseudo operating lines and equilibrium curve defined in such a manner as to permit application of the method at reflux ratios near the minimum as well as reflux ratios which are large compared to the minimum.

Multi-component systems are placed on the basis of the key components by the definitions:

$$x = \frac{X_{lK}}{\Sigma X_{Keys}}$$

$$y = \frac{Y_{lK}}{\Sigma Y_{Keys}}$$

The equilibrium curve and pseudo operating lines are determined by a calculation of the composition on the feed tray and the tray above the feed.

The proposed method requires fewer calculations than the method of Jenny[10] and eliminates the trial and error in the determination of the feed tray temperature.

The maximum error is about 5 percent.

Nomenclature appears on last page of article.

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components is defined as

$$x = \frac{X_{lK}}{X_{lK} + X_{hK}}$$

$$y = \frac{Y_{lK}}{Y_{lK} + Y_{hK}}$$

where

x = mole fraction of the light key in the liquid on a two-component basis
y = mole fraction of the light key in the vapor on a two-component basis
X = mole fraction in the liquid on a multicomponent basis
Y = mole fraction in vapor on a multicomponent basis

Subscripts:

$_{hK}$ = heavy key component
$_{lK}$ = light key component

then the points x_w and x_D

where subscript w = Bottoms
D = Overhead

are readily plotted on a McCabe-Thiele diagram.

The feed tray composition may then be calculated by noting that usually in the fractionating section a few trays below the condenser the *vapor* composition of the components lighter than the light key has been reduced to a constant value even though the liquid composition may be changing quite rapidly. Similarly, in the stripping section, a few trays from the reboiler the *liquid* composition of the components heavier than the heavy key has attained a constant value even though the vapor composition may be changing quite rapidly. At the pinches, the vapor and liquid composition becomes constant in each section.

From the equations of the operating lines and the above observations it follows that for components lighter than the light key

$$X_f = \frac{d}{V_n\left(K_f - \frac{L_n K_f}{V_n K_{f+1}}\right)} \qquad (21)$$

Note 1. If L_n/V_n is small compared to K_f then the ratio K_f/K_{f+1} may be assumed to be one without introducing appreciable error.

Similarly for the components heavier than the heavy key

$$X_f = \frac{w}{V_m\left(\frac{L_m}{V_m} - K_f\right)} \qquad (22)$$

Where

X = mole fraction in liquid
d = moles of component in overhead
V = moles of vapor up-flow
L = moles of liquid down-flow
w = moles of component in bottoms
K = equilibrium constant

Subscripts:

$_n$ = fractionating section
$_m$ = stripping section

A feed tray temperature is assumed by using the pinch temperatures, as set forth by Jenny,[11] as a guide. This assumed temperature need not be the optimum in order to establish accurately the operating lines and obtain the optimum feed tray. The liquid compositions on the feed tray for the light and heavy components are calculated by equations (21) and (22). The vapor compositions are calculated by

$$Y_f = K_f X_f$$

and the compositions of the keys obtained by simultation.

Calculations are then made to obtain

1) liquid composition of tray f + 1;
2) boiling point of liquid on tray f + 1;
3) vapor composition of keys on tray f — 1.

Then, by placing trays f, f + 1, and f — 1 on a two-component basis in the same manner as the bottoms and overhead, x_f, y_f, x_{f+1} and y_{f-1} are obtained and the pseudo operating lines can be drawn, since two points have been established on each operating line:

1) x_D and (y_f, x_{f+1}) for fractionating section.
2) x_w and (x_f, y_{f-1}) for stripping section.

From a boiling point calculation of the bottoms and a dew point of the overhead, the relative volatility of the keys is known at four points (bottom, tray f, tray f +1, and top) over the temperature range of the multicomponent system. The liquid composition on a two-component basis is also known at these four points. A smooth curve of relative volatility versus liquid composition (on a two-component basis) through the points (x_t, α_t), (x_{f+1}, α_{f+1}) and (x_w, α_w) will, for all practical engineering purposes, sufficiently define the equilibrium curve for the fractionating section. Similarly, a curve through the points (x_w, α_w), (x_f, α_f), and (x_t, α_t) will sufficiently define the equilibrium curve for the stripping section.

If the variation of the relative volatility with temperature is small near the feed tray temperature the boiling point calculation for tray f + 1 is unnecessary and only the liquid composition of the keys for tray f + 1 need be calculated.

The equilibrium curve is obtained from the relation

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

where α = relative volatility of the light key with reference to the heavy key.

The trays are then stepped off as on the conventional McCabe-Thiele diagram for a two-component system.

If the variation of the relative volatility is very small over the entire temperature range of the multicomponent system there is no necessity for the calculation of the boiling point of the bottoms and the dew point of the overhead and the determination of the number of trays becomes extremely simple.

Determination of Optimum Feed Tray for Case I:

The optimum feed tray is that tray which straddles the intersection of the pseudo operating lines.

Determination of Optimum Feed Tray Temperature for Case I:

For assumptions of feed tray temperatures over a range of several degrees the ratio of $\Sigma Y/\Sigma X$ for the keys does not change appreciably. The equilibrium constant for the light key is equal to $y\Sigma Y/x\Sigma X$. The ratio y/x is obtained from the equilibrium curve for the two-component system at the optimum feed tray. $\Sigma Y/\Sigma X$ for the keys is obtained from the feed tray composition calculation.

If the assumed feed tray temperature varies considerably from the calculated optimum, a second calculation of the feed tray composition may be made if a very accurate optimum feed tray temperature is desired. However, this large difference in tempera-

tures (assumed and optimum) will, in general, have no appreciable effect on the tray determinations.

Minimum Reflux:

For reflux ratios near the minimum, the keys may pass through a maximum concentration value as shown by rearrangement of the equations of the operating lines illustrated by Jenny.[11] If the pinch temperatures show that the keys pass through a maximum before reaching the feed tray for the stripping section, and the tray above the feed for the fractionating section, tray calculations must be made through these maximum values in order to establish the pseudo operating lines on the two component diagram.

Case II. The Vapor of the Feed Is Not in Equilibrium With the Feed Tray Liquid

The placing of the multicomponent system on a two-component basis is essentially the same as for Case I, but with the following adjustments:

1) Calculation of feed tray composition;

A temperature spread is assumed between the feed tray and the tray above, with the spread being equally distributed on either side of the pinch temperatures as illustrated by Jenny,[11] thus obtaining the first assumption of temperatures of the feed tray and the tray above.

As before, rearranging the operating lines and noting the *vapor* composition of the light components in the fractionating section and the *liquid* composition of the heavy components in the stripping section approach a constant value then for the light components.

$$v_{f+F} = \frac{d}{1 - \frac{L_n}{V_n K_{f+1}}} \qquad (23)$$

and for the heavy components

$$l_f = \frac{w}{1 - \frac{V_m K_f}{L_m}} \qquad (24)$$

where

v_{f+F} = mols of vapor from feed tray plus mols of vapor from feed for a light component

l_f = mols of heavy component in liquid on feed tray.

The composition of the light and heavy components on trays f and f+1 may be calculated from equations (23) and (24) and a material balance around the feed point. The composition of the keys is obtained by simultation.

2) Determination of operating lines

The point (y_f, x_{f+1}) no longer locates a point on the operating line for the fractionating section because this is not an equilibrium step directly from the feed tray. Therefore, calculations of the composition of the keys must be carried to tray f+2 such that (y_{f+1}, x_{f+2}) locates the pseudo operating line for the fractionating section.

As an alternate, the lowest point on the operating line for the fractionating section may be taken as (y'_f, x_{f+1})

Where y'_f = mole fraction of the light key component, on a two component basis, in the Vapor phase above the feed point and entering the tray above the feed.

Determination of Optimum Feed Tray for Case II:

The optimum feed tray will lie between that for an all liquid feed (feed tray straddles intersection of operating lines) and an all vapor feed (tray f+1 straddles intersection of operating lines).

Determination of Optimum Feed Tray Temperature for Case II:

The optimum feed tray temperature is calculated as for Case I.

EXAMPLE III

Case I. Assume vapor of feed in equilibrium with feed tray liquid.

Debutanizer reference.[16]

	Mols Feed	Mols Overhead	Mols Bottoms
C_3	1.0	1.0	....
C_4	40.0	39.4	0.6
C_5	23.0	0.4	22.6
C_6	16.0	....	16.0
C_7	12.0	....	12.0
C_8	8.0	....	8.0
	100.0	40.8	59.2

Equilibrium Flash on Feed: 220° F. 100 psia.

	$K\left(\frac{100\text{ psia.}}{220°\text{ F.}}\right)$	Mols Vapor	Mols Liquid
C_3	4.5	0.6	0.4
C_4	1.96	15.8	24.2
C_5	.93	5.4	17.6
C_6	.45	2.1	13.9
C_7	.21	0.8	11.2
C_8	.105	0.3	7.7
		25.0	75.0

Tower operates at 100 psia.

Dewpoint of Overhead

	Mols Vapor	$K_{145°}$	V/K
C_3	1.0	2.6	0.4
C_4	39.4	1.00	39.4
C_5	0.4	0.38	1.0
	40.8	....	40.8

Boiling point of bottoms

	Mols	$K_{278°}$	MK
C_4	0.6	3.1	1.9
C_5	22.6	1.60	36.2
C_6	16.0	0.86	13.8
C_7	12.0	0.45	5.4
C_8	8.0	0.25	2.0
	59.2	....	59.3

Reflux Ratio = 3 mols reflux per mole overhead

$L_n = 122.4$

$V_n = 163.2$

$\left(\frac{L}{V}\right)_n = 0.75$

Temp. = 199° F. when $K_{c5} = 0.75$

Approximate fractionating pinch temperature

$L_m = 197.4$

$V_m = 138.2$

$\left(\frac{V}{L}\right)_n = 1.333$

$\left(\frac{L}{V}\right)_m = 1.428$ Temperature = 182° F. when $K_{c4} = 1.428$

Approximate stripping pinch temperature.

Calculation of feed tray composition:

The feed tray temperature is, in general, larger than the stripping pinch temperature, modified of course, by the quantity of light components present. Since the quantity of light components for this case must be small, a feed tray temperature of 200° F. was assumed.

	K_{200}	$\left(\frac{L}{V}\right)_m - K_f$	$X_f = \frac{w}{V_m\left[\left(\frac{L}{V}\right)_m - K_f\right]}$	$K_f - \left(\frac{L}{V}\right)_n$	$X_f = \frac{d}{V_n\left[K_f - \left(\frac{L}{V}\right)_n\right]}$
C_3	3.98			3.23	.00189
C_4	1.689				
C_5	0.76				
C_6	0.355	1.073	0.1076		
C_7	0.159	1.269	0.0685		
C_8	0.078	1.350	0.0428		

STRIPPING SECTION			FRACTIONATING SECTION		
α	x	y	α	x	y
1.95	.05	.0934	2.30	0.50	.697
1.98	.10	.1805	2.38	0.60	.782
2.04	.20	.339	2.44	0.70	.850
2.10	.30	.474	2.51	0.80	.910
2.17	.40	.591	2.58	0.90	.959
2.23	.50	.690	2.61	0.95	.980
2.31	.60	.775			

	X_f	$Y_f = K_f X_f$
C_3	.00189	.00754
C_6	.1076	.0382
C_7	.0685	.0109
C_8	.0428	.00334
	.2208	.05998

$$X_4 + X_5 = 1 - .2208$$
$$1.689\,X_4 + 0.76\,X_5 = 1 - .05998$$

By simultation

$X_4 = 0.376$ $\quad Y_4 = 0.634$

$X_5 = 0.403$ $\quad Y_5 = 0.306$

Summarizing for feed tray:

	X_f	Y_f
C_3	.00189	.00754
C_4	.376	.634
C_5	.403	.306
C_6	.1076	.0382
C_7	.0695	.0109
C_8	.0428	.00334

Calculation of composition on tray f + 1: $\left(\frac{V}{L}\right)_n = 1.333$

	1.333 Y_f	$-0.333X_D$	$= X_{f-1}$	$K_{.80}$	KX_{f-1}	$KX_{Adj.}$
C_3	.0101	.0081	.0020	3.42	.0069	
C_4	.844	.322	.522	1.41	.7350	.735
C_5	.4075	.003	.404	.60	.2420	.242
C_6	.0510	.000	.0510	.27	.0138	
C_7	.0145	.000	.0145	.12	.0017	
C_8	.0044	.000	.0044	.055	.0002	
					.9996	

Calculation of keys on tray f − 1: $\left(\frac{L}{V}\right)_m = 1.428$

	$1.428X_f$	$- 0.428X_w$	$= Y_{f-1}$
C_4	.535	.0043	.531
C_5	.574	.163	.411
			.942

On a two-component basis:

$$\alpha = \frac{K_{c3}}{K_{c4}}$$

	α	
$x_D = .99$		$y_{f-1} = .5645$
$x_w = .0258$	1.94	
$x_t = 0.976$	2.63	$z_F = 0.635$
$x_f = 0.483$	2.22	
$x_{f+1} = 0.563$	2.35	

Figure 3 represents the plot of α vs x

From Figure 3 and $y = \frac{\alpha x}{1 + (\alpha - 1)x}$

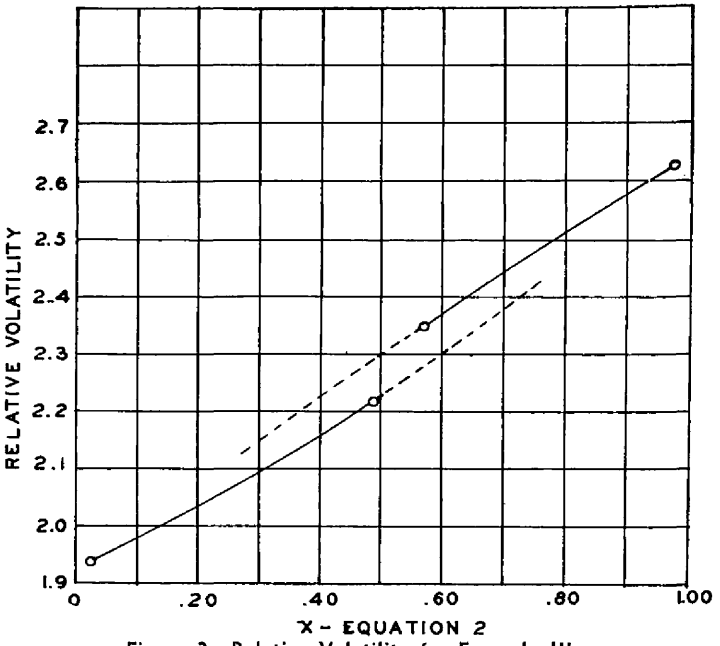

Figure 3—Relative Volatility for Example III.

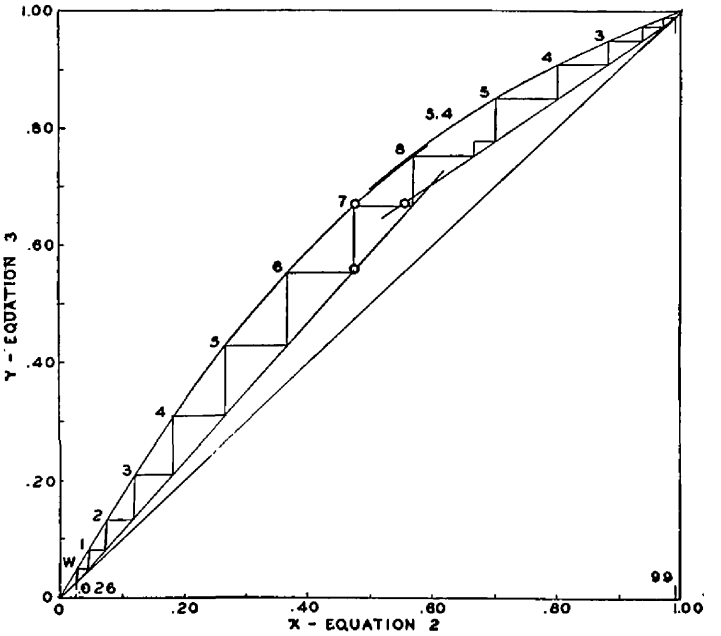

Figure 4—Determination of Trays for Example III.

The equilibrium curves are drawn on Figure 4 and the operating lines plotted from x_D and (x_{f+1}, y_f) and x_w and (y_{f-1}, x_f).

The trays are stepped off as on the conventional McCabe-Thiele[1] diagram.

Optimum Feed Tray:

Step that passes over intersection of the operating lines = 8th tray above reboiler.

Optimum Feed Tray Temperature:

From calculation of feed tray composition

$\Sigma X_{keys} = 0.779$
$\Sigma Y_{keys} = 0.940$

From Figure 4:

$y_f = 0.75$
$x_f = 0.57$

$$K_{c4} = \frac{(0.75)\ (0.940)}{(0.57)\ (0.779)} = 1.59 \text{ at optimum feed tray}$$

Temperature = 195° F.
From tray calculation = 195° F.

It may be noted that the feed tray composition was not calculated at the optimum temperature, but this had no effect on the final results.

EXAMPLE IV

Case II. The vapor portion of the feed is considered not in equilibrium with the feed tray liquid.

The following data were taken from Jenny's[11] article:

	Feed	Overhead	Bottoms
C_1	26	26.0	....
C_2	9	9.0	....
C_3	25	24.6	0.4
n-C_4	17	0.3	16.7
n-C_5	11	....	11.0
n-C_6	12	....	12.0
	100	59.9	40.1

Equilibrium Flash on Feed:

$$\left(\frac{V}{L}\right)_F = 2$$

	K_{175}	Liquid	Vapor
C_1	13.0	1	25
C_2	3.2	1	8
C_3	1.3	7	18
C_4	0.63	8	9
C_5	0.27	7	4
C_6	0.13	10	2
	....	34	66

Reflux Ratio = 1.5

Reboiler Temperature = 300° F.

	K	α
C_3	2.7	1.86
n-C_4	1.45	

Dewpoint of Overhead = 63° F.

	Y_D	K	α	X_t
C_3	.411	0.51	3.18	0.810
n-C_4	.005	0.16	....	0.032
	....	....	....	0.842

Feed Tray Temperature = 205° F.

	X_f	K	α	Y_f
C_3	.351	1.55	1.938	0.544
n-C_4	.404	0.80	....	0.323
	....	....	....	0.867

Tray f+1: Temperature = 160° F.

	1	K	α
C_3	39.0	1.14	2.11
C_4	35.8	.54	....
	74.8	....	....

	Tray f—1		Tray f+2
	Y_{f-1}		X_{f+2}
C_3	0.512	C_3	0.556
C_4	0.397	n-C_4	0.357
	0.909		0.913

On a Two-Component Basis:

	α
$x_D = 0.988$	....
$x_w = .0234$	1.86
$x_t = 0.96$	3.18
$x_f = 0.465$	1.938
$x_{f+1} = 0.521$	2.11
$x_{f+2} = 0.610$	....
$y_{f-2} = 0.564$	....
$z_F = 0.595$	....

Figure 5 is a plot of α vs. x. A smooth curve is drawn through (α_w, x_w), (α_f, x_f), and (α_t, x_t) for the stripping section equilibrium curve and through (α_w, x_w), (α_{f+1}, x_{f+1}), and (α_t, x_t) for the fractionating section equilibrium curve.

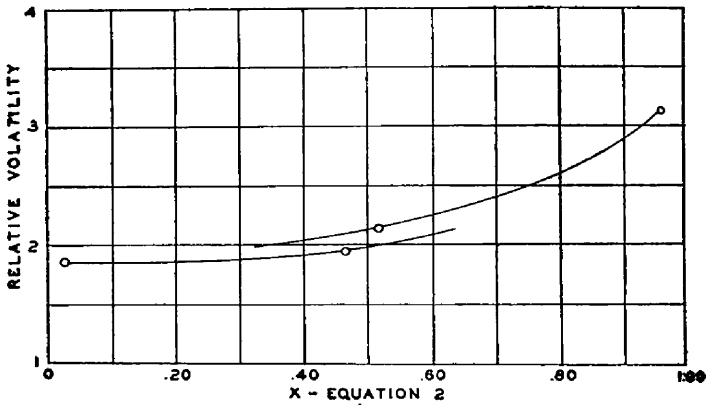

Figure 5—Relative Volatility for Example IV.

From Figure 5:

FOR STRIPPING SECTION			FRACTIONATING SECTION		
α	x	y	α	x	y
1.87	0.1	0.174	2.1	0.5	0.677
1.90	0.2	0.322	2.25	0.6	0.771
1.91	0.3	0.450	2.40	0.7	0.849
1.92	0.4	0.561	2.64	0.8	0.914
1.98	0.5	0.665	2.95	0.9	0.965
2.1	0.6	0.775	3.13	0.95	0.985

The graphical solution for the tray requirements is shown in Figure 6.

Optimum Feed Tray:

Since the feed was over 50 percent vaporized, the concentration of x_{f+1}, fell slightly below the intersection of the operating lines (discussed previously), and the point (y_f, x_{f+1}) fell between the two operating lines due to the type of feed tray action assumed.

Feed Tray Temperature:

The feed tray temperature is 205° F. since x_f on the graph corresponds to the value determined from the feed tray composition calculated using 205° F. as the assumed temperature.

EXAMPLE V

Determination of feed tray composition for the case of a split key.

The vapor of the feed is considered in equilibrium with the feed tray liquid.

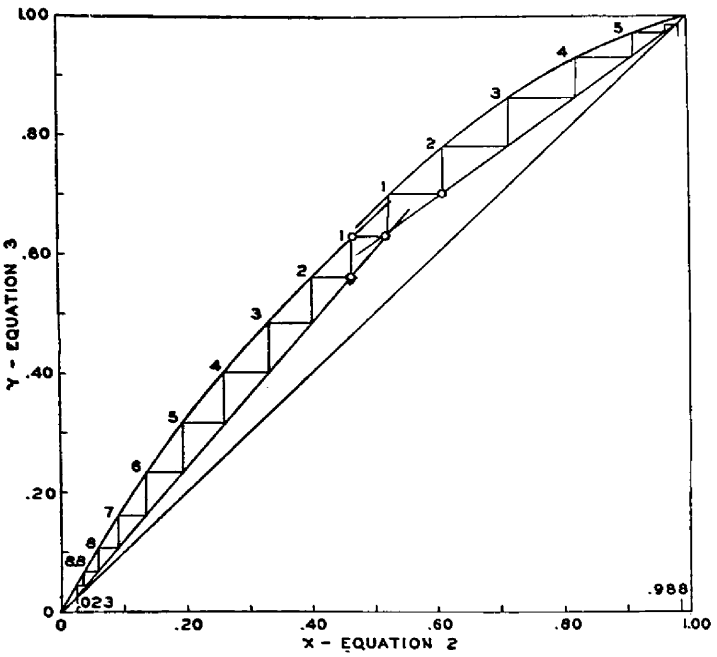

Figure 6—Determination of Trays for Example IV.

Depropanizer example of Jenny's[11] with split key.

Material Balance:

	Feed	Overhead	Bottoms
C_1	3	3.0	....
C_2	7	7.0	....
C_3	15	14.7	0.3
n-C_4	33	8.2	24.8
n-C_5	30	0.03	30.0
n-C_6	12	....	12.0
	....	32.9	67.1

Reflux Ratio = 1.75

$\frac{L_n}{V_n} = 0.635$ $\qquad$ $\frac{V_n}{L_n} = 1.575$

$\frac{L_m}{V_m} = 2.13$ $\qquad$ $V_n = 90.4$

$V_m = 59.4$

Tower pressure = 200 psia.

From Jenny's[11] calculations.

Reboiler Temperature = 265° F.

	MPH	K_{265}	MK
C_3	0.3	3.15	1.0
n-C_4	24.8	1.52	37.6
n-C_5	30.0	0.80	24.0
n-C_6	12.0	0.45	5.4
	67.1	....	68.0

Overhead: Temperature = 120° F.

	MPH	K_{120}	M/K	X_t
C_2	14.7	1.13	13.0	.388
n-C_4	8.2	0.46	17.8	.531
n-C_5	0.03	0.16	0.2	.006

Now if a heavy key is selected

$$hK = C_4 + C_5$$

in order to calculate the feed tray composition, a plot of K_{hK} vs. K_{C_4} will be a straight line as shown in Figure 7.

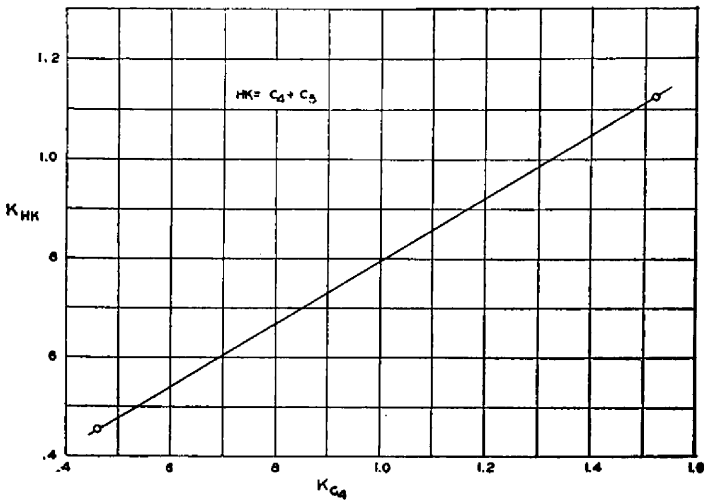

Figure 7—Definition of Equilibrium Constant—Example V.

The points for the plot are obtained as follows:

Top: $K_{C_4} = 0.46$ $\qquad$ $K_{hK} = \frac{8.23}{18.0} = 0.456$

Bottom: $K_{C_4} = 1.52$ $\qquad$ $K_{hK} = \frac{61.6}{54.8} = 1.125$

Calculation of Feed Tray Composition:

Assume Feed Tray temperatures = 200° F. and calculate the composition of the light and heavy components as in Example III.

	K_{200}	X_f	Y_f
C_1	22	.00156	.0343
C_2	5.3	.01661	.0880
C_3	2.08	*.1291	*.269
n-C_4	.98	*.476	*.466
n-C_5	.44	*.2707	*.1191
n-C_6	.22	.1060	.0233

* Calculation of concentration of C_3, n-C_4 and n-C_5.

From Figure 7: $K_{hK} = 0.785$ when $K_{C_4} = .98$

$X_3 + X_{hK} = 1 - (.00156 + .01661 + .1060) = .8758$

$2.08X_3 + 0.785X_{hK} = 1 - (.0343 + .0880 + .0233) = .8544$

By simultation:

$X_3 = .1291$ $\qquad$ $Y_3 = .269$

$X_{hK} = .7467$ $\qquad$ $Y_{hK} = .5854$

$X_4 + X_5 = .7467$

$.98X_4 + .44X_5 = .5854$

By simultation:

$X_5 = .2707$ $\qquad$ $Y_5 = .1191$

$X_4 = .476$ $\qquad$ $Y_4 = .466$

The tray requirements are then determined as in Examples IV and V.

The initial distribution of the intermediate key may be checked by using it as one of the keys on the same type diagram.

Discussion and Conclusions

The method presented offers a solution to the number of trays at any reflux ratio, optimum feed tray and optimum feed tray temperature with fewer calculations than are required by other methods of equal accuracy.

The greatest inaccuracy in the method lies in the determination of the equilibrium curve. However, even with very large variations of the relative volatility of the key components, the equilibrium curve is defined with sufficient accuracy to give the tray requirements with a maximum error of about five

percent. If the variation of the relative volatility of the key components is extremely large or erratic, a few calculations at the bottom of the tower, top of the tower, and around he feed point will serve to define the equilibrium curve with sufficient accuracy. However, in general, this is unnecessary.

The present method may be applied with equal accuracy to systems with a component which has a volatility intermediate between that of the keys. The initial distribution of the intermediate component may be checked by the graphical method if the intermediate component is selected as a key. However, distribution by the method of total reflux as outlined by Carey[13] is usually sufficiently accurate.

A number of examples, selected from the literature, are presented in Table 3. A wide variety of conditions are represented:

1) Up to 70 percent light components.
2) Up to 70 percent heavy components.
3) As many as 13 components.
4) Split keys.
5) Conditions of feed from all liquid to all vapor.
6) Relative volatility of the keys from 1.26 to 7.
7) Two-fold variation of the relative volatility of the key components from reboiler to overhead.

Case 8 in Table 3, which involved a split key with a large quantity of the intermediate component, small amounts of the key components, large variation of the relative volatility of the key components, and 13 components, demonstrates the broad application of the method.

The method is especially advantageous for those cases in which the feed tray concentration and temperature are necessary for a heat balance around the feed point.

For many systems the equilibrium curve does not change appreciably with a moderate change in reflux ratio. Thus, in design work, one equilibrium curve may suffice for several reflux ratios—the pseudo reflux ratio being determined by noting that over a limited range the ratio of the pseudo reflux ratio to the actual reflux ratio is constant.

TABLE 3
Comparison of Tray Calculations for Part III

PROBLEM	Reference	Method	Strip.	Trays Fract.	Total
1. Debutanizer	(16)	Author	8	5.4	13.4
		Calc.	8	5.6	13.6
2. Case B	(15)	Author	10.2	8.8	19.0
		Calc.	10.7	8.8	19.5
3. Case C	(15)	Author	9.5	10.2	19.7
		Calc.	9.3	10.1	19.4
4. Case E	(15)	Author	6.6	10.3	16.9
		Calc.	6.8	9.9	16.7
5. Case F	(15)	Author	7.2	9.2	16.4
		Calc.	7.2	9.2	16.4
6. Case G	(15)	Author	7.8	7.2	15.0
		Calc.	7.3	7.0	14.3
7. Phenol, O-cresol, etc	(14)	Author	13.5	13.0	26.5
		Calc.	13	13	26.0
8. Depropanizer, Stabilizer	(13)	Author	7.1	6.0	13.1
		Calc.	7 to 8	5 to 6	12 to 14
9. Depropanizer	(11)	Author	8.8	5.8	14.6
		Jenny	8.8	5.7	14.5
10. Depropanizer Split Key	(11)	Author	10.0	6.1	16.1
		Jenny	10.2	5.5	15.7

NOMENCLATURE

α = Relative volatility with respect to heavy key
d = Mols of component in overhead
D = Total mols overhead
f = Function
K = Equilibrium constant = Y/X
l = Mols of component in liquid phase
L = Mols of liquid downflow in column
m = Pseudo ratio of liquid to vapor
M = Mols of component
N = Number of theoretical trays
R = Reflux ratio, mols reflux per mole of overhead
R′ = Pseudo reflux ratio, mols reflux per mole of keys overhead
v = Mols of component in vapor phase
V = Mols of vapor upflow in tower
w = Mols of component in bottoms
W = Total mols of bottoms
x = Mol fraction of light key in liquid on two-component basis.
X = Mol Fraction of component in liquid phase
y = Mol fraction of light key in vapor on two-component basis.
Y = Mol fraction of component in vapor phase
z = Mol fraction of light key in vapor plus liquid on two-component basis
Z = Total mol fraction of component (liquid + vapor)

Subscripts:

D = Overhead
f = Feed tray
F = feed
h = heavy component, heavier than heavy key
hK = heavy key
i = intersection of operating lines
l = light component, lighter than light key
lK = light key
L = liquid
m = stripping section
M = minimum
n = fractionating section
t = top tray
V = vapor
w = bottoms

Superscripts:

′ = pseudo

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MINIMUM REFLUX RATIO—
THE COLBURN CORRELATION

CHAPTER II

Simplified Multi-Component Fractionation Calculations

RAYMOND V. BAILEY
and
JESSE COATES

***DISTILLATION** equipment represents a considerable segment of the total process plant investment, and the resolution of distillation process problems demands a large share of the energies of design and operating engineers. Distillation calculations for the lighter hydrocarbons involve complex algebraic type solutions, and it is common practice for process engineers to spend hours or even days in the determination of conditions about a single fractionating tower. This is especially noticeable when rigorous "tray-to-tray" type calculations are made. To speed up design and process control work various short-cut methods have been developed. Considerable progress has been made in this direction and this present article should prove a useful addition to this work.*

The authors are both connected with the College of Engineering, Louisiana State University, Baton Rouge, Bailey as a graduate student and Coates as professor of chemical engineering.

NOMENCLATURE

α = relative volatility with respect to the heavy key component
c = correction factor
d = mols of a given component appearing in the overhead
F = total mols of feed
K = equilibrium constant
l = mols of a given component in liquid phase
L = total mols of liquid downflow
ϕ = relative volatility with respect to the light key component $= \alpha/\alpha_{lk}$
ζ = empirical factor
q = total heat needed to convert one mole of feed into saturated vapor divided by the molal latent heat = approximately mol percent of liquid in the feed
r = ratio of mols of light key to heavy key component at pinch
R = reflux ratio, mols of liquid flowing in fractionating section per mole of overhead product
v = mols of a given component in the vapor phase
V = total mols of vapor upflow
w = total mols of a given component appearing in the bottoms

Subscripts

h = heavier than the heavy key component
hK = heavy key component
l = lighter than the light key component
lK = light key component
m = stripping pinch
M = minimum
n = fractionating pinch

UNTIL recently the problem of calculating the minimum reflux ratio has been time consuming and laborious. Several methods[1, 2, 4, 5, 6] have been proposed to simplify these calculations. Among these, the method of Colburn[2] is very accurate, but requires considerable time in application. The method of Underwood[5, 6] is rigorous for cases of constant relative volatilities and constant molal overflow. However, for many cases in which the relative volatility varies appreciably, the approximation of the temperature at which to evaluate the terms in Underwood's equations may lead to 10 to 20% error in the final results.

The modified Scheibel-Montross[4] method as presented by Bailey and Coates,[1] in general, appears to be as satisfactory as the Colburn correlation, so far as accuracy is concerned. However, it should be noted that the degree of separation of the key components should have some effect on the correction terms in the Bailey-Coates method. Insufficient allowance for this was made. For poor separations of the key components, the method gives an approximate answer, even though a good one for most cases. This method calls for the determination of a minimum reflux ratio for the separation of the key components.

On the other hand, the Colburn method is based directly on conditions

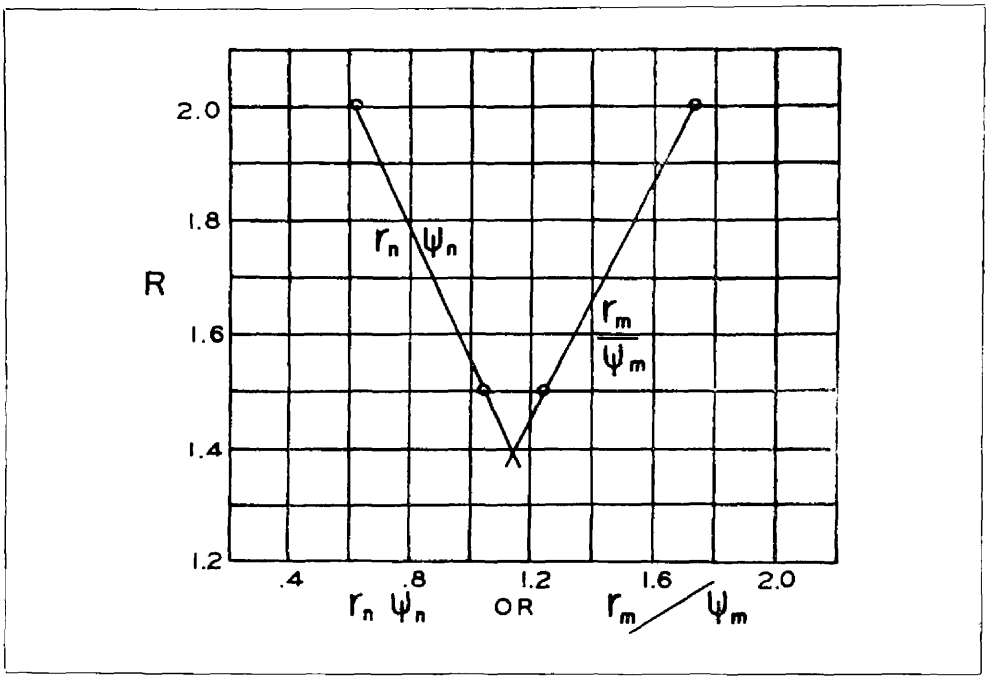

Figure 1—Determination of Minimum Reflux—Example I.

as they exist in multicomponent systems and it is unnecessary to place the system on a two-component basis. As a consequence, the Colburn method appears to be on a sounder basis. In addition, the use of the Colburn correlation is particularly advantageous for cases in which the assumption of constant molal overflow is not permissable. The direct evaluation of pinch compositions can be used for heat balances and partial compensation of non-constant molal overflow can be made. Therefore, a method of solving the Colburn relations at a saving of time over the usual method is desirable.

The method presented in this paper is a modified solution of the equations involved in the Colburn correlation which permits these relations to be satisfied with a considerable saving of time over that usually required. The time requirement for calculation compares favorably in all cases with the modified Scheibel-Montross method as presented by Bailey and Coates and in many cases the time requirement is reduced considerably, especially when the minimum reflux ratio is desired for several feed conditions for a given separation.

The Colburn criterium for minimum reflux ratio is divided into two parts, $r_n\psi_n$ and $\frac{r_m}{\psi_m}$, which, for a given separation, can be evaluated on the basis of the liquid flow in the fractioning and stripping pinches, respectively. Once $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ are evaluated for one reflux ratio, $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ can be readily approximated at another reflux ratio by the methods presented in this paper.

In many cases a plot of minimum reflux ratio versus feed conditions is desirable. Methods for making these plots from three easily determined points in each pinch are described in this paper.

Development of Equations:

If the equation of the operating line for the fractionating section is written in the form

$$l_{n+1} = v_n - d = \frac{V_n K_n}{L_n} l_n - d \qquad (1)$$

it may be noted that in the pinch

$$l_{n+1} = l_n$$

and equation (1) may be written

$$l_n = \frac{d}{\frac{V_n K_n}{L_n} - 1} \qquad (2)$$

Equation (2) may be employed to calculate the mols of the individual components at the fractionating pinch. Since the value of $\frac{V_n K_n}{L_n}$ is very close to one for the heavy key component, the heavy key component is generally obtained by difference rather than from equation (2).

Similarly, the mols of the individual components in the stripping section pinch may be obtained from the following equation:

$$l_m = \frac{w}{1 - \frac{V_m K_m}{L_m}} \qquad (3)$$

with the mols of the light key component being obtained by difference.

By noting that the fractionating pinch occurs when the heavy key component reaches its maximum concentration in that section, equation (1) may be arranged to give

$$K_{hk_n} = \left(1 + \frac{d_{hk}}{l_{hk_n}}\right) \frac{L_n}{V_n} \qquad (4)$$

and for sharp separations, since

$$1 + \frac{d_{hk}}{l_{hk_n}} \rightarrow 1$$

$$K_{hk_n} = \frac{L_n}{V_n} \text{ (Approx)} \qquad (5)$$

This relation may be employed for approximating the temperature of the fractionating pinch.

In a similar manner, by the application of equation (3) to the light key

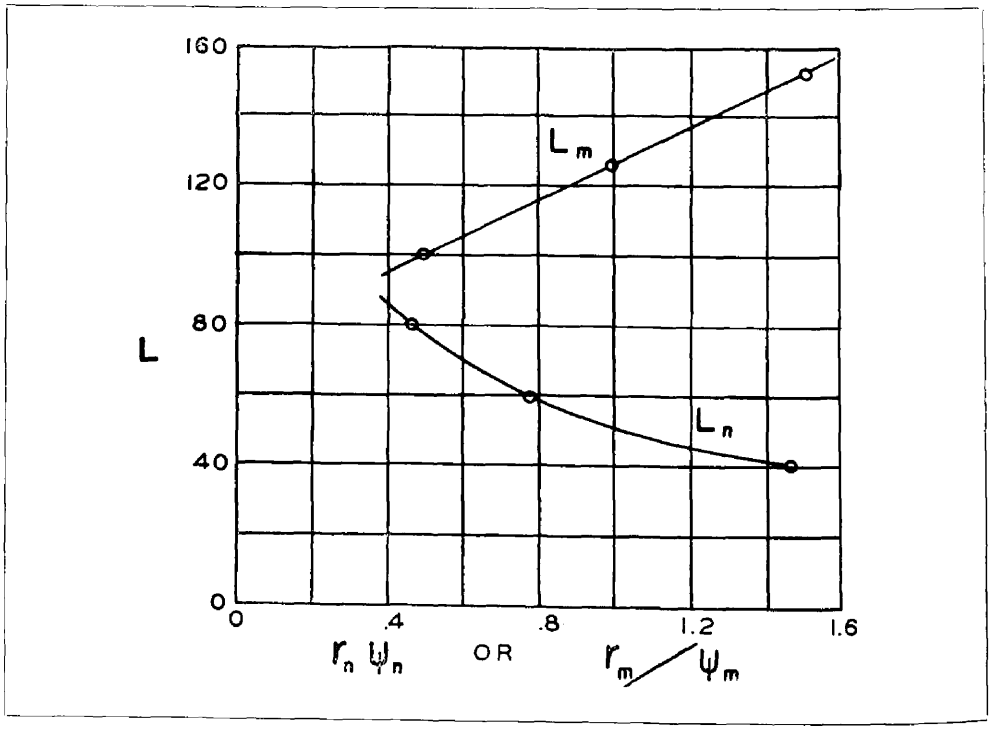

Figure 2—Example II. Liquid Flow—Pinch Ratio Relation.

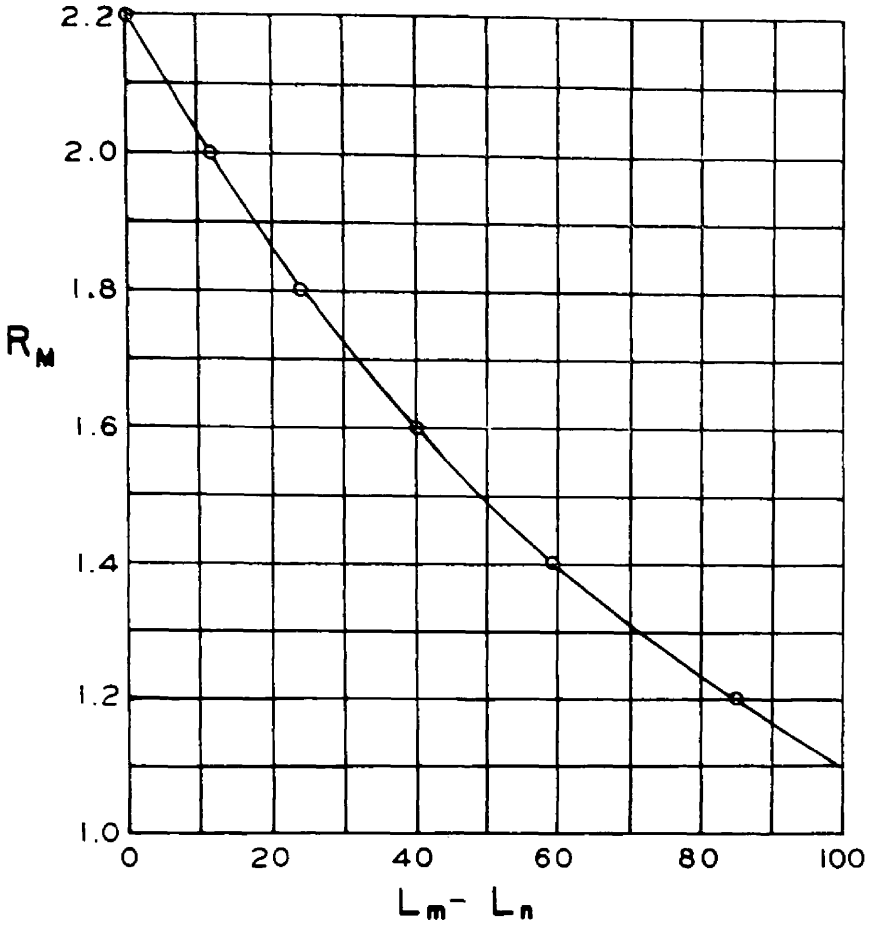

Figure 3—Minimum Reflux Ratio Versus Liquid in Feed—Example II.

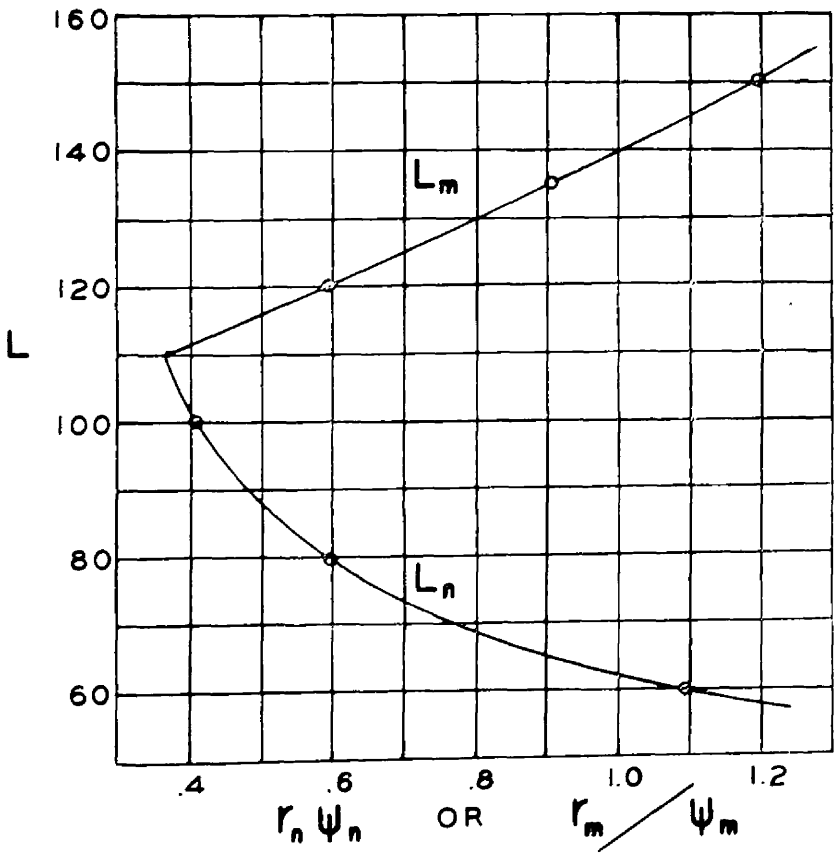

Figure 4—Example III. Liquid Flow—Pinch Ratio Relation.

component in the stripping pinch

$$K_{1k_m} = \left(1 - \frac{w_{1k}}{l_{1k_m}}\right) \frac{L_m}{V_m} \tag{6}$$

and

$$K_{1k_m} = \frac{L_m}{V_m} \text{ (Approx)} \tag{7}$$

Thus, a means is provided for approximating the pinch temperatures. The approximation may be corrected later, if necessary, by using equations (4) and (6).

In many cases, it is more convenient to use relative volatilities than equilibrium constants. By the substitution of $\frac{L_n}{V_n}$ from equation (4) into equation (2)

$$l_n = \frac{d}{\frac{K_n}{K_{hk_n}}\left(1 + \frac{d_{hk}}{l_{hk_n}}\right) - 1} = \frac{d}{\alpha - 1 + \frac{d_{hk}\alpha}{l_{hk_n}}} \tag{8}$$

For sharp separations

$$\frac{d_{hk}}{l_{hk_n}} \rightarrow 0$$

and

$$l_n = \frac{d}{\alpha - 1} \text{ (Approx)} \tag{9}$$

By similar treatment for the stripping pinch

$$l_m = \frac{w}{1 - \phi + \frac{w_{1k}\phi}{l_{1k_m}}} \tag{10}$$

or

$$l_m = \frac{w}{1 - \phi} \text{ (Approx)} \tag{11}$$

Colburn presented the following correlation for minimum reflux:

$$\frac{r_m}{r_n} = \psi \tag{12}$$

and if the factors, c_m and c_n, which were called for in Colburn's original method, are taken to be one

$$\psi = \frac{1}{\left(1 - \frac{\Sigma l_{1_n}}{L_n}\right)\left(1 - \frac{\Sigma \alpha l_{h_m}}{L_m}\right)} \tag{13}$$

The assumption of c_m and c_n equal to one has no appreciable effect on the results.

If ψ is broken down into two parts

$$\psi = \psi_n \psi_m \tag{14}$$

where

$$\psi_n = \frac{L_n}{L_n - \Sigma l_{1_n}} \tag{15}$$

$$\psi_m = \frac{L_m}{L_m - \Sigma \alpha l_{h_m}} \tag{16}$$

and applying the criterium of minimum reflux

$$\frac{r_m}{\psi_m} = r_n \psi_n \tag{17}$$

where $\frac{r_m}{\psi_m}$ and $r_n\psi_n$, for a given separation may be evaluated on the basis of the liquid flow in the stripping and

fractionating pinches respectively.

The expression $\Sigma\alpha l_{h_m}$ in equation (16) may be rearranged as follows, in order to eliminate the necessity of multiplying the mols of each heavy component by its respective relative volatility.

$$\Sigma\alpha l_{h_m} = \frac{\Sigma K_{h_m} l_{h_m}}{K_{hk_m}}$$

but

$$\Sigma K_{h_m} l_{h_m} = \left(\frac{L}{V}\right)_m (\Sigma l_{h_m} - \Sigma W_h)$$

Therefore

$$\Sigma\alpha l_{h_m} = \frac{\Sigma l_{h_m} - \Sigma W_h}{\frac{V_m K_{hk_m}}{L_m}} \qquad (18)$$

During the calculation of the mols of the heavy key component in the stripping pinch the term $\frac{V_m K_{hk_m}}{L_m}$ will be obtained as a natural result of the calculations.

Summarizing:

$$r_n\psi_n = \frac{l_{lk_n}}{l_{hk_n}} \left| \frac{L_n}{L_n - \Sigma l_{h_n}} \right. \qquad (19)$$

$$\frac{r_m}{\psi_m} = \frac{l_{lk_n}}{l_{hk_m}} \left| \frac{L_m - \left[\frac{\Sigma l_{h_m} - \Sigma W_h}{\left(\frac{VK_{hk}}{L}\right)_m}\right]}{L_m} \right. \qquad (20)$$

Application and Discussion of Equations:

The application of the equations will be illustrated for two cases: 1) A minimum reflux ratio is desired for a given separation and a single feed condition; and 2) a series of minimum reflux ratios is desired for a given separation and various feed conditions.

Case I. Minimum Reflux Ratio for A Given Separation and a Single Feed Condition—

An outline of the steps in the solution for this case follows:

1) Assume a reflux ratio and determine the approximate temperatures of the pinches using equations (5) and (7). If the temperature of the stripping pinch is lower than that of the fractionating pinch a lower reflux ratio should be selected, since the stripping pinch temperature must always be greater than that of the fractionating pinch for multicomponent systems.

2) By means of equations (2) and (3) or (9) and (11), whichever is more convenient, determine the approximate mols of the components in the pinches.

3) Correct the mols of the components in the pinches for the degree of separation of the key components. If the separation is relatively sharp or the relative volatilities are not changing appreciably with temperature at these points equations (8) and (10) may be used directly. However, if the separation is not sharp, the relative volatilities may vary between the approximate temperature and the true temperature of the pinch. In this case equations (4) and (6) are used to re-evaluate the temperatures, and equations (2) and (3) used to recalculate the pinch compositions.

4) By equations (19) and (20) evaluate $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ at the respective pinches

5) For any other reflux ratio, by assuming that only the mols of the light key component in the stripping pinch and the mols of the heavy key component in the fractionating pinch change with reflux ratio, approximate values of $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ are obtained by equations (19) and (20).

6) From a plot of reflux ratio versus $r_n\psi_n$ and $\frac{r_m}{\psi_m}$, determine the approximate minimum reflux from the intersection of the lines where

$$r_n\psi_n = \frac{r_m}{\psi_m}.$$

For relatively sharp separations, if the original reflux ratio, which was assumed, is within 50 percent of that determined in step (6). the reflux so determined will be within approximately two percent of the true minimum reflux ratio. However, in general, this intersection is not at the proper value of $r_n\psi_n$ or $\frac{r_m}{\psi_m}$. but the two are displaced in the same direction such that a very rapid convergence to the true minimum reflux ratio may be obtained.

7) Using the reflux ratio obtained from step (6) evaluate $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ precisely and obtain the true minimum reflux ratio as in step (6). Linear extrapolation is permissable since the reflux ratio from step (6) is close to the minimum.

Case II. A Series of Minimum Reflux Ratios Versus Feed Condition For a Given Separation—

Assume three liquid flows in each pinch. These liquid flows, at this point, are not related by any material balance and there are no formal rules for their selection. The best procedure is to alternate between the two pinches and plot $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ versus liquid flow as the calculations are made. By following this procedure the liquid flows in the respective pinches can be selected such that the curves overlap in the region of the feed condition range under consideration, thus, eliminating inaccurate extrapolation or calculation of extra points.

For poor separations, it is convenient to assume both the liquid flow in the pinch and the mols of the heavy key component for the fractionating pinch or the mols of the light key component for the stripping pinch in order to obtain faster convergence of the calculation and fewer adjustments.

Determine $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ for each liquid flow in the respective pinches. It may be noted at this point, that it is, in general, more convenient to use equations (4) and (6) to correct the liquid flow in the pinches rather than to correct the temperatures.

Plot the liquid flow versus $r_n\psi_n$ or $\frac{r_m}{\psi_m}$ for each pinch. From this plot select values of L_n and L_m at the point where $r_n\psi_n = \frac{r_m}{\psi_m}$. The value of L_n and L_m selected will correspond to a minimum reflux ratio for a feed condition of $L_m - L_n = qF$.

Three sample calculations are given to illustrate the application of the method to various types of systems.

Illustrative Example I

Case I: Minimum Reflux Ratio for Debutanizer[4] with 75 percent Liquid in Feed.

	Mols Feed	Mols Overhead	Mols Bottoms
C_3	1.0	1.0	....
C_4	40.0	39.4	0.6
C_5	23.0	0.4	22.6
C_6	16.0	....	16.0
C_7	12.0	....	12.0
C_8	8.0	....	8.0
		40.8	59.2

Pressure = 100 psia.
Equilibrium constants from Scheibel's[4] nomograph.
Assume $R_M = 2.0$
Then $L_n = 81.6$
$L_m = 81.6 + 75 = 156.6$

$\left(\frac{L}{V}\right)_n = .667 \qquad \left(\frac{L}{V}\right)_m = 1.61$

Fractionating Pinch—

	K^{190}	$\left(\frac{VK-1}{L}\right)$	l_1	K_{corr}^{191}	$\left(\frac{VK-1}{L}\right)_2$	l_2
C_3	3.60	4.4	.23	3.62	4.42	.23
C_4	1.51	1.26	31.2	1.52	1.265	31.1
C_5	.667	....	*50.2	.671	....	*50.3

* By Difference.

$$C_3 K_{corr} = \left(1 + \frac{0.4}{50.2}\right)(.667) = .671$$

$$r_n\psi_n = \frac{31.1}{50.3}\left|\frac{81.6}{81.6 - .2}\right. = .621$$

Stripping Pinch—

	K^{196}	$\left(\frac{VK}{L}\right)_1$	$\left(\frac{1-VK}{L}\right)_1$	l_1	K_{corr}^{195}	$\left(\frac{VK}{L}\right)_2$	l_2
C_4	1.61	....	....	*74.1	1.60	....	*74.1
C_5	.72	.446	.554	40.8	.715	.445	40.8
C_6	.33	.205	.795	20.1	.328	....	}
C_7	.148	.092	.908	13.2	.148	....	41.7
C_8	.07	.044	.956	8.4	.07	....	}

* By difference.

$$C_4 K_{corr} = \left(1 - \frac{.6}{74.1}\right)(1.61) = 1.60$$

$$\frac{r_m}{\psi_m} = \frac{74.1}{40.8}\left|\frac{156.6 - \frac{41.7 - 36}{.715}}{156.6}\right. = 1.73$$

From the above calculations it is seen that $R_M < 2.0$

If $R_M = 1.5 \quad L_n = 61.2 \quad L_m = 136.2$

$$r_n\psi_n \cong \frac{31.1}{61.2 - 31.3}\left|\frac{61.2}{61.2 - .2}\right. = 1.042$$

$$\frac{r_m}{\psi_m} \cong \frac{136.2 - 40.8 - 41.7}{40.8}\left|\frac{136.2 - \frac{5.7}{.715}}{136.2}\right. = 1.24$$

Plotting $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ versus reflux ratio in Figure 1, it is seen that the two intersect at $R_M = 1.39$.

Assuming $R_M = 1.39$ and repeating the above calculations

$$r_n\psi_n = 1.042$$

$$\frac{r_m}{\psi_m} = 1.06$$

If these points are plotted on Fig. 1, the intersection of $r_n\psi_n$ and $\frac{r_m}{\psi_m}$ gives $R_M = 1.38$.

It may be noted that this is the same value of minimum reflux ratio that was obtained by the original Colburn method using the correction factors in the ψ term.

This example illustrates the technique recommended for the determination of a minimum reflux ratio for a given separation and feed condition.

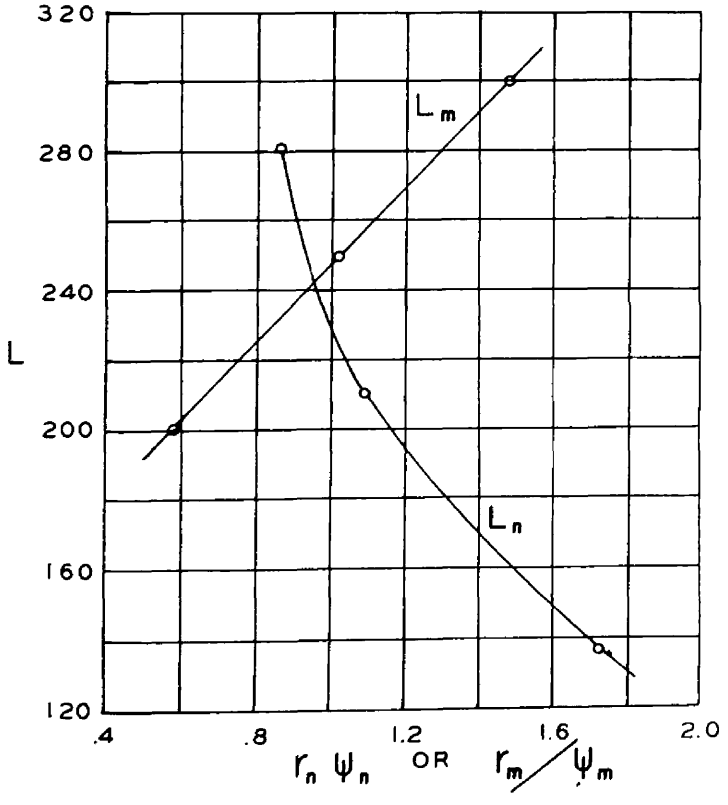

Figure 5—Example IV. Liquid Flow—Pinch Ratio Relation.

Illustrative Example II

Case II:

	Mols Feed	α	Mols Overhead	Mols Bottoms
A	25	4	25	....
B	25	2	25	trace
C	25	1	trace	25
D	25	0.5	....	25
			50	50

A plot of minimum reflux ratio versus percent liquid in feed is desired.

It may be noted that, for this sharp separation and constant relative volatility, the mols of A and B in the fractionating pinch and the mols of C and D in the stripping pinch are independent of reflux ratio if appreciable quantities of C and B are present in the respective pinches. The relative volatility need be constant only over the range of temperature covered by the pinches.

Fractionating Pinch—

	α	$\alpha - 1$	l_n
A	4	3	8.33
B	2	1	25
			33.33

$$L_n = 60\, r_n\psi_n = \frac{60}{60 - 8.33}\left|\frac{25}{60 - 33.33}\right. = 1.09$$

$$L_n = 80\, r_n\psi_n = \frac{80}{80 - 8.33}\left|\frac{25}{80 - 33.33}\right. = .595$$

$$L_n = 100\, r_n\psi_n = \frac{100}{100 - 8.33}\left|\frac{25}{100 - 33.33}\right. = .41$$

Stripping Pinch—

	ϕ	$1 - \phi$	l_m	$\alpha\, l_m$
C	.5	.5	50	
D	.25	.75	33.3	16.65
			83.3	

$$L_m = 120\frac{r_m}{\psi_m} = \frac{120 - 83.3}{50}\left|\frac{120 - 16.65}{120}\right. = .592$$

$$L_m = 135\frac{r_m}{\psi_m} = \frac{135 - 83.3}{50}\left|\frac{135 - 16.65}{135}\right. = .905$$

$$L_m = 150\frac{r_m}{\psi_m} = \frac{150 - 83.3}{50}\left|\frac{150 - 16.65}{150}\right. = 1.19$$

From these data, L_n, $r_n\psi_n$, L_m and $\frac{r_m}{\psi_m}$ the plot in Figure 2 was obtained.

From Figure 2 at points where $r_n\psi_n = \frac{r_m}{\psi_m}$

L_n	$\frac{L_n}{D}$	L_m	$L_m - L_n$ = % Liq. in Feed
60	1.2	144.5	84.5
70	1.4	128.5	58.5
80	1.6	120.0	40.0
90	1.8	115.0	25.0
100	2.0	112.0	12.0
110	2.2	110.0	0.0

From these data, the plot, Figure 3, of R_M versus percent liquid in the feed was obtained.

This example illustrates the extreme simplicity of obtaining a plot of minimum reflux ratio versus feed condition for a sharp separation of the key components if the relative volatilities are essentially constant over the temperature range covered by the pinch temperatures.

Illustrative Example III

Case II: Constant Relative Volatility, Poor Separation of Key Components.

	Mols Feed	α	Mols Overhead	Mols Bottoms
A	25	4	25	....
B	25	2	23	2
C	25	1	2	23
D	25	0.5	....	25
			50	50

Problem: Obtain a plot of minimum reflux ratio versus percent liquid in the feed.

For a case of this type, it is simple to use equations (8) and (10). Values of l_{hk_n} and l_{lk_m} are assumed and the corresponding L_n, $r_n\psi_n$, L_m and $\frac{r_m}{\psi_m}$ determined.

Fractionating Pinch—

Assume $l_{hk_n} = 30$

	(1) α	(2) $\alpha - 1$	(3) $\frac{d_{hk}\,\alpha}{l_{hk_n}}$	(2)+(3)	l_n
A	4	3	.267	3.267	7.65
B	2	1	.134	1.134	20.3
C	1				30
					$L_n = 57.95$

$$r_n\psi_n = \frac{20.3}{30}\left|\frac{57.95}{57.95 - 7.65}\right. = .78 \text{ for } L_n = 57.95$$

This was repeated for two other values of l_{hk_n}. The stripping section was handled in a similar manner and the plots made as in Example II.

The results are as follows:

Fractionating Section—

l_{hk_n}	L_n	$r_n\psi_n$
50	79.21	.474
15	40.27	1.47
30	57.95	.78

Stripping Section—

l_{lk_m}	L_m	$\frac{r_m}{\psi_m}$
25	100.1	.504
50	127.1	.993
75	152.9	1.505

From plot of $r_n\psi_n$ versus L_n and $\frac{r_m}{\psi_m}$ versus L_m

L_n	L_m	$r_n\psi_n = \frac{r_m}{\psi_m}$	% Liquid = $L_m - L_n$ In Feed	$R_M = \frac{L_n}{D}$
80	98	.465	18	1.6
60	114	.75	54	1.2
50	126	.97	76	1.0

This example illustrates the elimination of trial and error for a poor separation of the key components if the relative volatility of the components are essentially independent of temperature over the range covered by the pinch temperatures.

Illustrative Example IV

Case II, Deisobutanizer

	Mols Feed	Mols Overhead	Mols Bottoms
C_3	1.4	1.4	....
i-C_4	48.0	47.96	.04
n-C_4	36.1	11.3	24.8
n-C_5	3.4	....	3.4
n-C_6	11.1	....	11.1
		60.66	39.34

Tower pressure = 110 psia.
Equilibrium constants from Ref. (3).
(NOTE—Continue with "Fractionating Pinch," above, next column.)

Fractionating Pinch—

For this poor separation of the key components, trial and error is kept to a minimum by assuming $l_{n\text{-}c_4}$ and correcting the temperature and total liquid flow to correspond to the assumed value of $l_{n\text{-}c_4}$. Since the relative volatility of i-c_4 to n-c_4 will be of the order of 1.3 the mols of i-c_4 in the fractionating pinch will be of the order of 100.

Assume $l_{n\text{-}c_4} = 100$. Then $L_n \cong 200$.

$$\text{Then } \left(\frac{L_n}{V_n}\right)_1 = \frac{200}{260.66} = .766$$

$$K_{n\text{-}c_4} = \left(1 + \frac{11.3}{100}\right)(.766) = .854$$

Temperature = 137° F.

	K^{137}	$\frac{VK-1}{L}$	l_n	K^{139}	$\frac{VK-1}{L}$	l_n	$r_n\psi_n$
C_3	2.25	1.94	.72	2.25	1.9	.72	
i-C_4	1.10	.436	110.	1.12	.44	109.	
n-C_4	.854		100.	.866		100.	
			$L_n = 210.72$			$L_n = 209.72$	1.091

$$\left(\frac{L_n}{V_n}\right)_2 = \frac{210.72}{271.38} = .778$$

$$K_{n\text{-}c_4} = \left(1 + \frac{11.3}{100}\right)(.778) = .866$$

Temperature = 139° F.

$$r_n\psi_n = \frac{109}{100}\left|\frac{209.7}{209}\right. = 1.091$$

If $l_{n\text{-}c_4} = 50$ $L_n \cong 50 + 109.7 \cong 160$

$$\left(\frac{L_n}{V_n}\right)_1 = \frac{160}{220.66} = .725$$

$$K_{n\text{-}c_4} = \left(1 + \frac{11.3}{50}\right)(.725) = .889$$

Temperature = 144° F.

	K^{144}	$\frac{VK-1}{L}$	l_n	K^{138}	$\frac{VK-1}{L}$	l_n	$r_n\psi_n$
C_3	2.3	2.17	.65	2.2	2.18	.64	
i-C_4	1.135	.569	84.5	1.08	.561	85.5	
n-C_4	.889		50.	.848		50.	
			$L_n = 135.15$			$L_n = 136.14$	1.71

$$\left(\frac{L_n}{V_n}\right)_2 = \frac{135.15}{195.81} = .691$$

$$K_{n\text{-}c_4} = \left(1 + \frac{11.3}{150}\right)(.691) = .848$$

Temperature = 138° F.

(NOTE—Continue reading at top of next column.)

If $l_{n\text{-}c_4} = 150$ $L_n \cong 150 + 110 \cong 260$

$$\left(\frac{L_n}{V_n}\right)_1 = \frac{260}{320.66} = .81$$

$$K_{n\text{-}c_4} = \left(1 + \frac{11.3}{150}\right)(.81) = .87$$

Temperature = 141° F.

	K_{141}	$\frac{VK}{L}$	l_n	K_{143}	$\frac{VK-1}{L}$	l_n	$r_n \psi_n$
i-C_3	2.25	1.78	.79	2.3	1.80	.8	
i-C_4	1.11	.376	129.8	1.130	.371	129.2	
n-C_4	.87		150.	.885		150.	
			$L_n = 280.59$			$L_n = 280.0$	.861

$$\left(\frac{L_n}{V_n}\right)_2 = \frac{280.6}{341.3} = .824$$

$$K_{n\text{-}c_4} = \left(1 + \frac{11.3}{150}\right)(.824) = .885$$

Temperature = 143° F.

Stripping Pinch—

Since the separation of the key components is very sharp.

$$K_{1\text{-}c_4} = \frac{L_m}{V_m}$$

$$L_m = 200 \quad \frac{L_m}{V_m} = K_{1\text{-}c_4} = \frac{200}{200 - 39.34} = 1.24$$

Temperature = 152° F.

	K_{152}	$\frac{VK}{L}$	$\frac{1-VK}{L}$	l_m	$\frac{r_m}{\psi_m}$	$\frac{17.8-14.5}{200 - .786}$
i-C_4	1.24			*66.2	66.2	
n-C_4	.975	.786	.214	116.	116	= .582
n-C_5	.39	.314	.686	5.0		
n-C_6	.165	.133	.867	12.8		
				$L_m = 200$		

* By difference.

$$L_m = 250 \quad \frac{L_m}{V_m} = K_{1\text{-}c_4} = \frac{250}{211.7} = 1.182$$

Temperature = 147° F.

	K_{147}	$\frac{VK}{L}$	$\frac{1-VK}{L}$	l_m	$\frac{r_m}{\psi_m}$
i-C_4	1.182			*118.5	
n-C_4	.925	.782	.218	113.9	
n-C_5	.36	.304	.696	4.9	
n-C_6	.15	.127	.873	12.7	
				$L_m = 250.$	1.023

* By difference.

$$L_m = 300 \quad \frac{L_m}{V_m} = K_{1\text{-}c_4} = \frac{300}{261.7} = 1.149$$

Temperature = 144° F.

	K_{141}	$\frac{VK}{L}$	$\frac{1-VK}{L}$	l_m	$\frac{r_m}{\psi_m}$
i-C_4	1.149			*169.8	
n-C_4	.895	.78	.22	112.8	
n-C_5	.34	.296	.704	4.8	
n-C_6	.14	.122	.878	12.6	
				$L_m = 300$	1.485

* By difference.

From a plot, Figure 5, of L_n versus $r_n\psi_n$ and L_n versus $\frac{r_m}{\psi_m}$

L_n	L_m	$r_n \psi_n = \frac{r_m}{\psi_m}$	% Liquid = $L_m - L_n$ In Feed	$R_M = \frac{L_n}{D}$
242	242	.96	0.0	3.63
220	252	1.05	28.0	3.30
200	263.5	1.15	63.5	3.00
190	270	1.21	80.0	2.85
180	278	1.28	98.0	2.70

This typical deisobutanizer example illustrates the method of application of the equations to a system in which the relative volatility of the components are not constant and the separation of the key components is very poor. It may be noted, for the fractionating pinch, that a very rapid convergence and a minimum of trial and error is obtained by assuming the mols of $l_{n\text{-}c_4}$ in the pinch and adjusting the temperature and total liquid flow to correspond to this assumption.

Conclusions

The method of calculation presented offers a rapid, accurate solution for minimum reflux. It is especially advantageous for the determination of minimum reflux versus feed condition for a given separation. It may be noted that, in general, a minimum reflux for a given feed condition is best determined by first obtaining the curve of minimum reflux versus feed condition. This is best illustrated by Example III where trial and error is completely eliminated for the determination of a plot of R_M versus feed condition.

Further, as pointed out by Colburn, it should be noted that the correlation holds for those cases with a component having a volatility intermediate between that of the key components, provided the distribution of the intermediate component can be estimated. However, further work is needed in order to be able to rapidly and accurately predict the distribution of intermediate components.

For non-ideal mixtures in which the minimum reflux ratio might be limited by a tangent, stepwise calculations must be made to check the minimum reflux ratio obtained by Colburn's correlation.

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CHAPTER III

SIMPLIFIED MULTI-COMPONENT FRACTIONATION CALCULATIONS

Distribution of Split Keys

ABSTRACT:

The application of Underwood's (7,8,9) equations and the Colburn (2) correlation for minimum reflux for the determination of the distribution of split keys at minimum reflux is presented. Equations have been developed to systematize the calculations and minimize the trial and error involved in the application of the Colburn correlation and Underwood's equations.

A study has been made of the distribution of split keys which will give the optimum number of trays at reflux ratios other than total and minimum. The distribution of split keys obtained at total reflux was found to give a minimum number of trays at all reflux ratios except those very close to the minimum. At this point the optimum distribution approaches that obtained at minimum reflux.

INTRODUCTION:

In multicomponent systems it is necessary to specify the maximum quantity of one component in the overhead and the maximum quantity of a second component in the bottoms. These specified components are known as the key components. The specified component with the highest volatility is designated the light key component and the other component is called the heavy key component. A heavy component is one which has a volatility less than the heavy key component and which appears in the fractionating pinch in negligible quantity. Similarly, a light component is one which has a volatility greater than that of the light key component and which appears in the stripping pinch in negligible quantity. A split key is defined as an unspecified component which appears in appreciable quantities in both pinches. Usually the relative volatility of a split key component is intermediate between that of the two specified components.

In order to determine the minimum reflux for a system containing split keys the distribution of these split keys in the overhead and bottoms must be determined. Underwood (7,8,9) has developed equations for the determination of minimum reflux for multicomponent systems and has demonstrated the application of these equations to systems containing split keys. The application is given here in slightly different form for purposes of comparison and to illustrate the use of Newtion's (4)

method to reduce the trial and error involved in the solution of the equations. An attempt is made to apply the equations to systems containing split keys in which the relative volatility is not constant. However, the accuracy of Underwood's equations depends on a choice of the feed tray temperature if the relative volatilities are not constant. In many cases the variation of the relative volatilities is sufficiently large that considerable doubt as to the true minimum reflux exists after the application of the Underwood equations due to the difficulty involved in selecting a good value for the feed tray temperature.

Colburn (2) presented an empirical correlation for minimum reflux which minimizes the doubt as to the proper temperatures to use. Colburn has stated that the distribution of the split key component at minimum reflux is such that the ratio of the mols of the split key component in the fractionating pinch to that in the stripping pinch lies between the corresponding ratios of the light key component and the heavy key component. However, for large values of Colburn's empirical term, ψ , there would be a considerable range of distributions of the split key component which would satisfy this criterium. In addition, a tremendous amount of trial and error is encountered in trying to satisfy Colburn's criteria.

Bailey and Coates (1) have simplified the calculations required for Colburn's correlation for cases in which there are no split keys. Equations are presented in this article for the application of Colburn's correlation to split keys.

Previously, the Fenske (3) equation for total reflux has been used to estimate the distribution of split keys for tray calculations for all reflux ratios between the minimum and total. No previous study has been made in an attempt to determine the distribution of split keys which would give an optimum number of trays for a given reflux ratio and separation of the key components.

APPLICATION OF UNDERWOOD'S EQUATIONS FOR THE DISTRIBUTION OF SPLIT KEYS AT MINIMUM REFLUX:

Underwood has derived the following equations for the determination of minimum reflux ratio:

$$\sum \frac{\alpha Z_F}{\alpha - \phi} = 1 - q \qquad (1)$$

$$\sum \frac{\alpha X_D}{\alpha - \phi} = R_M + 1 \qquad (2)$$

where α - relative volatility of a component with respect to the heavy key component.

X - mol fraction of a component in the liquid phase.

Z - total mol fraction of a component (liquid plus vapor).

q - heat required to convert one mole of feed to saturated vapor divided by the latent heat of the feed.

R - mols of reflux per mol of overhead.

ϕ - defined by equation (1) and the value of ϕ lies between the relative volatilities of the key components.

Subscripts:

D - overhead
F - feed
M - minimum

Since the distribution of the split key is unknown, it is more convenient to define the system by stating the mols of the light key component appearing in the overhead and the mols of the heavy key component appearing in the bottoms rather than specifying the mol fractions, respectively.

Rewriting equations (1) and (2) in terms of mols

$$\sum \frac{\alpha M_F}{\alpha - \phi} - M_V = 0 \qquad (3)$$

$$\sum \frac{\alpha d}{\alpha - \phi} = (R_M + 1) D = V_n \qquad (4)$$

Where M_F - mols of a component in the feed.
M_V - mols of vapor in the feed.
d - mols of a component in the overhead.
D - total mols of overhead.
V_n - total mols of vapor upflow in the fractionating section of the tower.

If N split keys are present in the feed then there are N plus one values of ϕ which lie between the relative volatilities of the key components that will satisfy equation (3). By substituting these N plus one values of ϕ in equation (4) there are obtained N plus one equations which on simultation yield the distribution of each split key and the minimum reflux.

In order to facilitate the solutions of equation (3) it is proposed that Newton's (4) method for irrational roots be used.

$$\phi_2 = \phi_1 - \frac{f(\phi_1)}{f'(\phi_1)} \qquad (5)$$

Where ϕ_1 - first assumption of ϕ.
ϕ_2 - second approximation of ϕ.

$$f(\phi_1) = \sum \frac{\alpha M_F}{\alpha - \phi_1} - M_V$$

$$f'(\phi_1) = \sum \frac{\alpha M_F}{(\alpha - \phi_1)^2}$$

Procedure:

The procedure for application of Underwood's equations to systems containing split keys and constant volatility is as follows:

1. Assume a value of ϕ between the relative volatilities of the light key component and the split key component.
2. Correct this assumption by means of equation (5) until equation (3) is satisfied.
3. Repeat steps (1) and (2) for a value of ϕ between the relative volatilities of the heavy key component and the split key component.
4. Substitute the values of ϕ obtained into equation (4) and simultate to obtain the distribution of the split key and the minimum reflux.

Quite often, from observation of the system, a fair choice of ϕ_1 can be made which will give $\phi_2 = \phi$ for most purposes.

Varying Relative Volatility:

The proper temperature for the evaluation of relative volatilities is the feed tray temperature. For the case in which light and

heavy components are absent this temperature is readily determined from the thermal condition of the feed. However, if light and/or heavy components are present the temperature of the feed tray is not readily obtainable and the use of arithmetic averages of the relative volatilities taken at the pinch temperatures is recommended. These temperatures are obtained at the expense of further trial and error. If the variation of the relative volatility is appreciable the equations of Underwood appear to be unreliable. For this case, the use of the Colburn correlation, as presented later, is recommended.

Recommended Procedure:

The recommended procedure for the application of Underwood's equations to systems containing split keys and varying relative volatility is as follows:

1. Assume a reasonable minimum reflux and distribution of the split key.
2. Determine the approximate temperatures of the pinches by use of equations (7b) and (8b) which appear in the next part of this article.
3. Evaluate the arithmetic average relative volatilities from the relative volatilities obtained at these pinch temperatures.
4. Proceed as for constant volatility using these average relative volatilities.
5. If the minimum reflux ratio and distribution of

the split key differs appreciably from the assumed values, repeat the calculations using the calculated values.

The following examples have been selected to illustrate the application of Underwood's equations for constant relative volatility and for varying relative volatility.

Illustrative Example I.

Application of Underwood's equations to a system with constant relative volatility:

Component	α	Mols Feed	d	w
A	4	15	15	—
B	2	15	15	trace
C	1.7	20	d_c	w_c
D	1.3	20	d_d	w_d
E	1.0	15	trace	15
F	0.5	15	—	15
		100		

Feed is saturated vapor. Components C and D are split keys.

	αM_F	$\alpha - \phi$ ($\phi = 1.9$)	$\frac{\alpha M_F}{\alpha - \phi}$	$\frac{\alpha M_F}{(\alpha-\phi)^2}$	$\alpha - \phi$ ($\phi = 1.9018$)	$\frac{\alpha M_F}{\alpha - \phi}$	$\frac{\alpha d}{\alpha - \phi}$
A	60	2.1	28.6	13.6	2.098	28.6	28.6
B	30	0.1	300.	3000.	.0982	305.5	305.5
C	34	-0.2	-170.	850.	-.2018	-168.7	-8.43 d_c
D	26	-0.6	-43.3	72.2	-.602	-43.2	-2.16 d_d
E	15	-0.9	-16.7	18.5	-.902	-16.7	----
F	7.5	-1.4	-5.35	3.8	-1.402	-5.4	----
			93.2	3958.1		100.1	V_n

$\phi = 1.9 - (93.2 - 100)/3958.1 = 1.9018$

	αM_F	$\frac{\phi=1.5}{\alpha-\phi}$	$\frac{\alpha M_F}{\alpha-\phi}$	$\frac{\alpha M_F}{(\alpha-\phi)^2}$	$\frac{\phi=1.508}{\alpha-\phi}$	$\frac{\alpha M_F}{\alpha-\phi}$	$\frac{\alpha d}{\alpha-\phi}$
A	60	2.5	24	9.6	2.492	24.0	24.0
B	30	0.5	60	120.	.492	61.0	61.0
C	34	0.2	170	850.	.192	177.0	8.85 d_c
D	26	-0.2	-130	650	-.208	-125.0	-6.25 d_d
E	15	-0.5	-30	60.	-.508	-29.5	———
F	7.5	-1.0	-7.5	7.5	-1.08	-6.9	———
			86.5	1697.1		100.6	V_n

$$\phi = 1.5 - (86.5 - 100)/1697.1 = 1.508$$

	$\frac{\phi=1.1}{\alpha-\phi}$	$\frac{\alpha M_F}{\alpha-\phi}$	$\frac{\alpha M_F}{(\alpha-\phi)^2}$	$\frac{\phi=1.11}{\alpha-\phi}$	$\frac{\alpha M_F}{\alpha-\phi}$	$\frac{\alpha d}{\alpha-\phi}$
A	2.9	20.7	7.1	2.89	20.8	20.8
B	.9	33.3	37.0	.89	33.7	33.7
C	.6	56.6	94.5	.59	57.6	2.88 d_c
D	.2	130.0	650.	.19	136.9	6.84 d_d
E	-.1	-150.0	1500.	-.11	-136.2	———
F	-.6	-12.5	20.8	-.61	-12.3	———
		78.1	2309.4		100.5	V_n

$$\phi = 1.1 - (78.1 - 100)/2309.4 = 1.11$$

Equating V_n's

$$28.6 + 305.5 - 8.43\, d_c - 2.16\, d_d = 24.0 + 61.0 + 8.85\, d_c - 6.25\, d_d$$

$$24.0 + 61.0 + 8.85\, d_c - 6.25\, d_d = 20.8 + 33.7 + 2.88\, d_c + 6.84\, d_d$$

From which $d_c = 16.81$; $d_d = 10.0$

$$R_M = \frac{28.6 + 305.5 - (8.43)(16.81) - (2.16)(10.0)}{15 \quad 15 \quad 16.81 \quad 10.0} - 1$$

$$= 3.00 - 1 = 2.00$$

Illustrative Example II: Application of Underwood's equations when relative volatility is not constant.

	M_F	d	w	
C_1	3	3.0	—	$q = .69$
C_2	7	7.0	—	Tower pressure = 200 psia
C_3	15	14.7	0.3	Equilibrium data from nomo-
C_4	33	*13.0	*20.0	graph by Scheibel (5).
C_5	30	0.2	29.8	C_4 is the split key.
C_6	12	—	12.0	
		37.9	62.1	

Assume $R_M = .75$

Then $L_n = (.75)(37.9) = 28.4$ $\quad L_m = 28.4 + 69 = 97.4$

$V_n = (1.75)(37.9) = 66.3$ $\quad V_m = 66.3 - 31 = 35.3$

$K_{hk_n} = (L/V)_n = .428$ Temp.= 196 F.

$K_{lk_m} = (L/V)_m = 2.76$ Temp.= 237 F.

	K^{196}	α^{196}	K^{237}	α^{237}	α_{av}
C_1	21.0	49.0	24.5	37.7	43.4
C_2	5.42	12.68	6.85	10.52	11.6
C_3	2.16	5.05	2.76	4.25	4.65
C_4	.948	2.22	1.30	2.00	2.11
C_5	.428	1.00	.65	1.00	1.00
C_6	.20	.47	.329	.51	.49

	M_F	α_{av}	αM_F	$\phi = 3.8$ $\frac{}{\alpha - \phi}$	$\frac{\alpha M_F}{\alpha - \phi}$	$\frac{\alpha M_F}{(\alpha-\phi)^2}$	$\phi = 3.712$ $\frac{}{\alpha - \phi}$	$\frac{\alpha M_F}{\alpha - \phi}$
C_1	3	43.4	130.	39.6	3.28	.1	39.688	3.28
C_2	7	11.6	81.2	7.8	10.4	1.3	7.888	10.3
C_3	15	4.65	69.7	.85	82.0	96.5	.938	74.4
C_4	33	2.11	69.5	-1.69	-41.1	24.3	-1.602	-43.3
C_5	30	1.00	30.0	-2.8	-10.71	3.8	-2.712	-11.05
C_6	12	.49	5.88	-3.31	-1.78	.5	-3.222	-1.82
					42.09	126.5		31.81

$\phi = 3.8 - (42.09 - 31)/126.5 = 3.712$

* Assumed distribution

	$\frac{\alpha M_F}{(\alpha-\phi)^2}$	$\phi = 3.705$ $\alpha-\phi$	$\frac{\alpha d}{\alpha-\phi}$		$\phi = 1.3$ $\alpha-\phi$	$\frac{\alpha M_F}{\alpha-\phi}$	$\frac{\alpha M_F}{(\alpha-\phi)^2}$
C_1	0.1	39.695	3.28		42.1	3.09	0.1
C_2	1.3	7.895	10.3		10.3	7.88	0.8
C_3	79.2	.945	72.3		3.35	20.8	6.2
C_4	27.0	-1.595	-1.322	d_{c4}	.81	85.8	106.
C_5	4.1	-2.705	-.07		-.30	-100.	333.3
C_6	.5	-3.215	----		-.81	-7.25	9.0
	112.2		V_n			10.32	455.4

$\phi = 3.712 - (31.81 - 31)/112.2 = 3.705$

$\phi = 1.3 - (10.32 - 31)/455.4 = 1.345$

	$\phi = 1.345$ $\alpha-\phi$	$\frac{\alpha M_F}{\alpha-\phi}$	$\frac{\alpha M_F}{(\alpha-\phi)^2}$	$\phi = 1.350$ $\alpha-\phi$	$\frac{\alpha d}{\alpha-\phi}$	
C_1	42.05	3.09	0.1	42.05	3.09	
C_2	10.25	7.92	0.8	10.25	7.92	
C_3	3.305	21.05	6.4	3.30	20.7	
C_4	.765	90.9	118.8	.76	2.78	d_{c4}
C_5	-.345	-86.95	252.	-.35	-.57	
C_6	-.855	-6.87	8.0	-.86	----	
		29.14	386.1		V_n	

$\phi = 1.345 - (29.14 - 31)/386.1 = 1.350$

Equating V_n's and solving $d_{c4} = 13.3$

Substituting in equation (4) $R_M = .787$

Note: If results had differed very much from assumptions, it would have been necessary to obtain a new set of average relative volatilities and repeat the calculations.

COLBURN CORRELATION FOR DISTRIBUTION OF SPLIT KEYS AT MINIMUM REFLUX:

For systems containing split keys Colburn (2) has shown that

1. $r_m/r_n=\psi$ at minimum reflux.

   where r_m - ratio of the mols of the light key component to the heavy key component in the stripping pinch.
   r_n - ratio of the mols of the light key component to the heavy key component in the fractionating pinch.
   ψ - empirical factor defined by equation (11a).

2. The distribution of the split key is such that the ratio of the mols of the split key component in the fractionating pinch to that in the stripping pinch lies between the corresponding ratios of the light key component and the heavy key component.

However, for large values of ψ, there would be a considerable range of distributions of the split key component which would satisfy criterium (2). In addition, a tremendous amount of trial and error is encountered in trying to satisfy both conditions (1) and (2) without a straightforward procedure which gives a rapid convergence to the true values.

In an attempt to surmount these difficulties it has been assumed that for the key components there exists a linear relation of $(\alpha-1)$ versus the ratio of the mols of the component in the fractionating pinch to that in the stripping pinch. In addition, the following equations have been developed in order to facilitate calculations.

For sharp separations of the key components in systems containing no components lighter than the light key component or heavier than the heavy key component the distribution of any intermediate components is given by

$$d_s = \frac{M_{s_F} \Big/ \alpha_s - 1}{\alpha_s \Big/ \alpha_{lK} - 1} \left\{ \frac{d_{lK}}{M_{lK_p}} \left[\alpha_{lK} - \frac{m}{m+1} (\alpha_{lK} - \alpha_s) \right] \right.$$

$$\left. + \frac{d_{hK}}{M_{hK_p}} \left[1 + \frac{m}{m+1} (\alpha_s - 1) \right] \right\} \qquad (6)$$

where $m = \dfrac{M_L - \Sigma M_{hF}}{M_V - \Sigma M_{lF}}$

α - relative volatility with respect to the heavy key component.
d - mols of a component overhead.
m - pseudo ratio of liquid to vapor.
M - mols.

Subscripts:
F - feed
h - heavy component
hK - heavy key component
l - light component
lK - light key component
L - liquid in feed
s - split key component
V - vapor in feed

A good first approximation for the distribution of split keys for any system may be obtained by the application of equation (6).

By rearrangement of the equations of the operating lines at the pinches

$$K_{hK_n} = \left(1 + \frac{d_{hK}}{l_{hK_n}}\right) \left(\frac{L}{V}\right)_n \qquad (7a)$$

$$K_{hK_n} \cong \left(\frac{L}{V}\right)_n \qquad (7b)$$

$$K_{lK_m} = \left(1 - \frac{w_{lK}}{l_{lK_m}}\right) \left(\frac{L}{V}\right)_m \qquad (8a)$$

$$K_{lK_m} \cong \left(\frac{L}{V}\right)_m \qquad (8b)$$

$$l_n = \frac{d}{\left(\frac{VK}{L}\right)_n - 1} \qquad (9)$$

$$l_m = \frac{w}{1 - \left(\frac{VK}{L}\right)_m} \qquad (10)$$

where K - equilibrium constant.
l - mols of a component in the liquid phase.
L - total mols of liquid downflow in tower.
V - total mols of vapor upflow in tower.
w - mols of a component appearing in the bottoms.

Subscripts:
m - stripping section
n - fractionating section

The empirical factor, ψ, in Colburn's correlation is given by

$$\psi = \frac{L_n \; L_m}{(L_n - \Sigma c_l \, l_{l_n})(L_m - \Sigma c_h \alpha_h \, l_{hm})} \qquad (11a)$$

where c_l and c_h are correction factors given in graphical form in Colburn's article.

In many cases no serious error is encountered if the

correction factors c_l and c_h are taken as unity. The expression can then be written in a more convenient form.

$$\psi = \frac{L_n \; L_m}{(L_n - \Sigma l_{l_n}) \; L_m - \dfrac{l_{hm} - \Sigma w_{hm}}{\left(\dfrac{VK_{hk}}{L}\right)_m}} \qquad (11b)$$

where $\left(\dfrac{VK_{hk}}{L}\right)_m$ is obtained of a necessity in the calculations of the pinch compositions.

By noting that the mols of all components in the pinches, except the heavy key component in the fractionating pinch and the light key component in the stripping pinch, change only slightly with reflux ratio and that ψ is practically constant

$$l'_{hk_n} = \frac{F_3 + \sqrt{(F_3)^2 + 4F_4\psi}}{2} \qquad (12)$$

and

$$l'_{lk_m} = l'_{hk_n} - F_3 \qquad (13)$$

where $F_3 = (l_{hk_m} + \Sigma l_{h_m}) - (l_{lk_n} + \Sigma l_{l_n}) - M_L$

$F_4 = (l_{ek_n})(l_{ak_m})$

Superscript (') denotes values corresponding to assumed values of d_s.

The correction in the mols of the split key overhead in order to meet the criterium of a linear relation for the key components of $(\alpha - 1)$ versus the ratio of the mols of the component in the fractionating pinch to that in the stripping pinch is then given by

$$\Delta d_s = \frac{F_1 w'_s - d'_s}{1 + F_1 + F_2 \left(\dfrac{d'_s}{l'_{hk_n} + l'_{lk_m}}\right)} \qquad (14)$$

where

$$F_1 = \left(\frac{l_{lk_n}}{l_{lk_m}}\right) \left[\frac{\left(\frac{VK_s}{L}\right)_n - 1}{1 - \left(\frac{VK_s}{L}\right)_m}\right]\left[\psi - (\psi - 1)\frac{\left(\frac{VK_s}{L}\right)_n - 1}{\left(\frac{VK_{lk}}{L}\right)_n - 1}\right]$$

$$F_2 = \frac{1}{\left(\frac{VK_s}{L}\right)_n - 1} + \frac{1}{1 - \left(\frac{VK_s}{L}\right)_m}$$

The correspondingly corrected mols of the heavy key component in the fractionating pinch, light key component in the stripping pinch, liquid flow in the fractionating pinch, and minimum reflux in order that $\frac{r_m}{r_n}$ still equal ψ are

$$l_{hk_n} = l'_{hk_n} - \sum \frac{F_2 \ (\Delta d_s)}{1 + \left(\frac{l_{lk_m}}{l_{hk_n}}\right)'} \tag{15}$$

$$l_{lk_m} = l'_{lk_m} + \sum \frac{F_2 \ (\Delta d_s)}{1 + \left(\frac{l_{hk_n}}{l_{lk_m}}\right)'} \tag{16}$$

$$L_n = \sum l_n + \sum \frac{\Delta d_s}{\left(\frac{VK_s}{L}\right)_n - 1} \tag{17}$$

$$R_M = \frac{L_n}{D' + \sum \Delta d_s} \tag{18}$$

Even though the list of equations appears quite lengthy and complicated, it should be noted that the expressions in most of the

equations are obtained in the process of calculating the pinch compositions and that the calculations proceed quite rapidly.

Application of Equations:

By use of equation (6) and approximate relative volatilities a first approximation of the split key distribution is obtained. A minimum reflux ratio is then assumed such that the temperature of the stripping pinch is slightly greater than the temperature of the fractionating pinch, the temperatures being obtained by means of equations (7b) and (8b). After applying equation (9) to all components lighter than the heavy key component and equation (10) to all components heavier than the light key component the value of ψ is obtained from equation (11). A first approximation of the mols of the heavy key component in the fractionating pinch and the light key component in the stripping pinch is obtained by means of equations (12) and (13), respectively. Then, from the application of equations (14), (15), (16), (17), and (18), corrected values of the distribution of the split key component, mols of the heavy key component in the fractionating pinch, mols of the light key component in the stripping pinch, liquid flow in the fractionating pinch and minimum reflux ratio are obtained. Using this new value of minimum reflux ratio and equations (7a) and (8a) to determine the temperatures at the pinches, the preceding calculations are repeated until the desired convergence is obtained. For most pusposes the second trial gives sufficiently precise results.

The method is illustrated for constant volatility and for varying volatility by the same illustrative examples which were solved by Underwood's equations.

Illustrative Example III:

As an example of the application of Colburn's correlation to a system of constant relative volatility, the following problem will be used.

Component	α	Mols Feed	d	w
A	4	15	15	--
B	2	15	15	trace
C	1.7	20	*17	*3
D	1.3	20	*9.96	*10.04
E	1.0	15	trace	15
F	0.5	15	--	15
		100	56.96	43.04

Feed is saturated vapor. Components C and D are split keys. Approximation of distribution of C and D by equation (6).

$$m = \frac{0 - 15}{100 - 15} = -.1765$$

$$m/(m+1) = -.1765/(1 - .1765) = -.214$$

$$d_c = \frac{(20)\,(0.7)\,[2 + (.214)\,(.3)]}{(1.7)\,(1.0)} = 17.0$$

$$d_D = \frac{(20)\,(.3)\,[2 + (.214)(.7)]}{(1.3)\,(1.0)} = 9.96$$

It may be noted that for this sharp separation of the key components that $\left(\frac{VK}{L}\right)_n - 1 = \alpha - 1$ and $1 - \left(\frac{VK}{L}\right)_m = 1 - \frac{\alpha}{\alpha_{1K}}$

* From equation (6)

Fractionating Pinch:

	$(VK/L) - 1$	l_n
A	3	5.0
B	1	15.0
C	0.7	24.3
D	0.3	33.2
E	—	l_{n_E}
F	—	—
		$77.5 + l_{n_E}$

Stripping Pinch:

	$1 - (VK/L)$	l_m
A	—	—
B	—	l_{m_B}
C	.15	20
D	.35	28.7
E	.50	30.
F	.75	20.
		$98.7 + l_{m_B}$

Assume $l_n = L_m = 110$

Then $$\psi = \frac{110}{110 - 5} \Big| \frac{110}{110 - (20 - 15)/.5} = 1.15$$

$$F_3 = 98.7 - 77.5 - 0 = 21.2$$

$$F_4 = (15)(30) = 450$$

Then $$l'_{n_E} = \frac{21.2 + \sqrt{(21.2)^2 + (4)(450)(1.15)}}{2} = 35.65$$

$$l'_{m_B} = 35.65 - 21.2 = 14.45$$

Then $$F_{1c} = (15/14.45)(.7/.15)\left[1.15 - (.7)(.15)\right] = 5.06$$

$$F_{1D} = (15/14.45)(.3/.35)\left[1.15 - (.3)(.15)\right] = .985$$

$$F_{2c} = 1/.7 + 1/.15 = 8.10$$

$$F_{2D} = 1/.3 + 1/.35 = 6.19$$

Then by equation (14)

$$\Delta d_c = \frac{(5.06)(3) - 17}{1 + 5.06 + (8.1)(17)/50.1} = -0.2$$

$$\Delta d_D = \frac{(.985)(10.04) - 9.96}{1 + .985 + [(6.19)(9.96)/50.1]} = -0.01$$

By equation (15)

$$l_{n_E} = 35.65 + \frac{.2 + .01}{1 + (14.45/35.65)} = 35.8$$

By equation (17)

$$L_n = 77.5 + 35.8 - (.2/.7) - (.01/.3) = 113.0$$

By equation (18)

$$R_M = \frac{113.0}{56.96 - .21} = 1.99$$

$$d_c = 17.0 - .2 = 16.8$$

$$d_D = 9.96 - .01 = 9.95$$

Further corrections are not essential since there was such a small change in the distribution of the split keys.

Illustrative Example IV: As another example of the application of the Colburn correlation the following depropaniser problem will be used.

	Mols Feed	d	w
C_1	3	3.0	—
C_2	7	7.0	—
C_3	15	14.7	0.3
C_4	33	*13.0	*20.0
C_5	30	0.2	29.8
C_6	12	—	12.0
	100	37.9	62.1

$q = .69$

Tower pressure = 200 psia

Equilibrium data from nomograph by Scheibel (5).

* First approximation from equation (6).

Assume $R_M = 0.75$

Then $K_{hK_n} = 0.75/1.75 = 0.428$ by equation (7b)

Temperature of fractionating pinch = 196 F.

Use 196 F. as temperature to evaluate α's for equation (6).

	K^{196}	α
C_3	2.16	5.05
C_4	.948	2.21
C_5	.428	1.00

Then by application of equation (6)

$$m = \frac{69 - 12}{31 - 10} = 2.71$$

$$d_{c4} = \frac{(33)(1.21)}{(2.21)(4.05)} \left\{ \frac{14.7}{15.0} \left[5.05 - \frac{(2.71)(5.05 - 2.21)}{3.71} \right] + \frac{0.2}{30} \left[1 + \frac{(2.71)(2.21 - 1)}{3.71} \right] \right\} = 13.0$$

Then $w_{c4} = 33 - 13 = 20$

Using $R_M = 0.75$

$L_n = (0.75)(37.9) = 28.4$ $\qquad L_m = 28.4 + 69 = 97.4$

$V_n = (1.75)(37.9) = 66.3$ $\qquad V_m = 66.3 - 31 = 35.3$

$K_{hK_n} \cong (L/V)_n = .428$ $\qquad$ Temperature = 196 F.

$K_{lK_m} \cong (L/V)_m = 2.76$ $\qquad$ Temperature = 237 F.

Fractionating Pinch: **Stripping Pinch:**

	K^{196}	$\frac{VK}{L}$	$\frac{VK}{L} - 1$	l_n	K^{237}	$\frac{VK}{L}$	$1 - \frac{VK}{L}$	l_m
C_1	21.1	49.0	48.0	.0625	—	—	—	—
C_2	5.42	12.68	11.68	.600	—	—	—	—
C_3	2.16	5.05	4.05	3.625	2.76	—	—	l_{1K_m}
C_4	.948	2.22	1.22	10.65	1.30	.471	.529	37.8
C_5	.428	—	—	l_{hK_n}	.65	.236	.764	39.0
C_6	—	—	—	—	.329	.119	.881	13.6
				$14.94 + l_{hK_n}$				$90.4 + l_{1K_m}$

From equation (11b)

$$\psi = \frac{28.4}{28.4 - .663} \Big| \frac{97.4}{97.4 - (1.6/.236)} = 1.10$$

Using equation (12)

$$F_3 = 90.4 - 14.94 - 69 = 6.46$$

$$F_4 = (3.625)(39) = 141.2$$

$$l'_{hK_n} = \frac{6.46 + \sqrt{(6.46)^2 + (4)(141.2)(1.10)}}{2} = 16.13$$

$$l'_{1K_m} = 16.13 - 6.46 = 9.67$$

Using equation (14)

$$F_1 = (3.625/9.67)(1.22/.529)\left[1.10 - (1.22)(.10)/4.05\right] = .935$$

Then $F_2 = 1/1.22 + 1/.529 = 2.71$

$$\Delta d_{04} = \frac{(.935)(20) - 13.0}{1 + .935 + (2.71)(13)/25.8} = 1.7$$

From equation (15)

$$l_{hK_n} = 16.13 - \frac{(2.71)(1.7)}{1 + (9.67/16.13)} = 13.25$$

From equation (16)

$$l_{1K_m} = 9.67 + \frac{(2.71)(1.7)}{1 + (16.13/9.67)} = 11.40$$

From equation (17)

$$L_n = 14.94 + 13.25 + (1.7/1.22) = 29.58$$

From equation (18)

$$R_M = 29.58/(37.9+1.7) = 0.746$$

Using $R_M = .746$, $d_{84} = 14.7$ for next trial

$$L_n = (.746)(39.6) = 29.6 \qquad L_m = 29.6 \quad 69 = 98.6$$

$$V_n = (1.746)(39.6) = 69.2 \qquad V_m = 69.2 - 31 = 38.2$$

$$(L/V)_n = .426 \qquad (L/v)_m = 2.58$$

$$K_{hK_n} = [1 + (.2/13.25)](.426) = .434 \quad \text{Temp.} = 197\ F.$$

$$K_{lK_m} = [1 - (.3/11.4)](2.58) = 2.51 \quad \text{Temp.} = 222\ F.$$

Fractionating Pinch: Stripping Pinch:

	K^{197}	$\frac{VK}{L}$	$\frac{VK}{L} - 1$	l_n	K^{222}	$\frac{VK}{L}$	$1 - \frac{VK}{L}$	l_m
C_1	21.0	49.2	48.2	.0625	----	---	----	---
C_2	5.4	12.68	11.68	.600	----	---	----	---
C_3	2.15	5.05	4.05	3.625	2.51	---	----	l_{lK_m}
C_4	.95	2.22	1.22	12.05	1.15	.446	.554	33.0
C_5	.434	---	---	l_{hK_n}	.56	.217	.783	38.0
C_6	----	---	---	---	.28	.109	.891	13.5
				$16.34 + l_{hK_n}$				$84.5 + l_{lK_m}$

$$\psi = \frac{29.6}{29.6 - .66} \Big| \frac{98.6}{98.6 - (1.5/.217)} = 1.10$$

$$F_3 = 84.5 - 16.34 - 69 = -.84$$

$$F_4 = (3.625)(38) = 138$$

$$l'_{hK_n} = \frac{-.84 + \sqrt{(.84)^2 + (4)(138)(1.10)}}{2} = 11.88$$

$$l'_{lK_m} = 11.88 + .84 = 12.72$$

$$F_1 = (3.625/12.72)\ (1.22/.554)\ [1.10 - (1.22/4.05)\ (.10)] = .672$$

$$F_2 = 1/1.22 + 1/.554 = 2.63$$

$$d_{c4} = \frac{(.672)\ (18.3) - 14.7}{1 + .672 + (2.63/24.6)\ (14.7)} = -.74$$

$$l_{hK_n} = 11.88 + \frac{(2.63)\ (.74)}{1 + (12.72/11.88)} = 12.82$$

$$l_{lK_m} = 12.72 - \frac{(2.63)\ (.74)}{1 + (11.88/12.72)} = 11.71$$

$$L_n = 16.34 + 12.82 - (.7/1.22) = 28.59$$

$$R_M = 28.59/(39.6 - .7) = .734$$

$$d_{c4} = 14.7 - .74 = 13.96$$

Repeating the calculations again

$$R_M = 0.740$$

$$d_{c4} = 14.04$$

DISTRIBUTION OF SPLIT KEYS FOR OTHER REFLUX RATIOS:

For any reflux ratio there is an optimum feed tray location or ratio of the key components at the feed tray which will give a minimum number of trays for that reflux ratio and a given separation of the key components. For a system containing split keys it is necessary to specify the distribution of the split keys between the overhead and bottoms before tray calculations can be made. This is in effect a specification of the feed tray location or ratio of the key components at the feed tray since there is only one point at which the concentrations of all components can be matched after the distribution of the split key has been specified. Thus, it is necessary to use trial and error in the distribution of the split keys until the concentrations can be matched at the optimum feed tray location if the optimum number of trays is to be obtained very precisely.

It has been general practice to distribute the split key by means of the Fenske equation for total reflux

$$S = \frac{\log \left[\frac{d_{lK}}{w_{lK}} \middle| \frac{w_{hK}}{d_{hK}} \right]}{\log \alpha_{lK}} = \frac{\log \left[\frac{d_s}{w_s} \middle| \frac{w_{hK}}{d_{hK}} \right]}{\log \alpha_s} \qquad (19)$$

where S - number of theoretical steps required at total reflux.
The relative volatilities are geometric means of the values taken at the condenser and reboiler.

and use this distribution for all other reflux ratios. However, no study has been made previously to determine if this is an optimum distribution.

Thus, we have two points where the distribution of the split key can be determined; total reflux and minimum reflux. Usually these two distributions are considerably different. In an effort to determine if the distribution of split keys for optimum trays at reflux ratios other than minimum or total was intermediate between these two extremes the data in Table II was compiled by tray to tray calculations. From this table the following observations can be made:

1. For all practical purposes the distribution of the split keys at total reflux will give an optimum number of trays for all reflux ratios except those which are extremely close to the minimum.
2. Using the distribution of the split key at total reflux, the ratio of the key components at the feed tray matches with fair precision the optimum ratio of the key components as given by the equations of Scheibel and Montross (6).

The above observations may be utilized to obtain reliable product compositions and optimum feed tray locations.

An illustrative example of the calculation of the distribution of a split key at total reflux follows.

Illustrative Example V: Determination of the distribution of a split key component at total reflux.

	Mols Feed	d	w	
C_1	3	3.0	—	Tower pressure = 200 psia
C_2	7	7.0	—	
C_3	15	14.7	0.3	Equilibrium constants
C_4	33	*13.0	*20.0	from nomograph by
C_5	30	0.2	29.8	Scheibel (5).
C_6	12	—	12.0	
	100	37.9	62.1	

	K140	d/K	α_T	K265	wK	α_w	$\alpha_{av} = \sqrt{\alpha_T \alpha_w}$
C_1	16.5	.18					
C_2	3.7	1.89					
C_3	1.39	10.58	6.61	3.3	.99	3.93	5.09
C_4	.55	23.6	2.62	1.59	31.8	1.892	2.22
C_5	.21	.95	1.00	.84	25.0	1.00	1.00
C_6				.45	5.4		
		37.20			63.19		

By equation (19)

$$\frac{\log\ (14.7)\ (29.8)/(.3)(.2)}{\log\ 5.09} = \frac{\log\ (d_{c4}/w_{c4})\ (29.8/.2)}{\log\ 2.22}$$

Then $d_{c4}/w_{c4} = .527$

$w_{c4} = 33/1.527 = 21.6$

$d_{c4} = 33 - 21.6 = 11.4$

* Assumed

TABLE IA

Comparison of Values of R_m and d_s at R_m

Problem	Feed Composition						Relative Volatilities					Feed Condition
	l	lk	s	hk	h	α_l	α_{lk}	α_s	α_{hk}	α_h		q
1	25	25	25	25	—	4	2	1.5	1.0	—		1.0
2	—	25	25	25	25	—	2	1.5	1.0	0.5		1.0
3	—	25	25	25	25	—	2	1.5	1.0	0.8		1.0
4	40	15	20	25	—	6	2.2	2.0	1.0	—		0.0
5	25	25	25	25	—	4	2	1.5	1.0	—		0.535
6	25	25	25	25	—	2.5	2	1.5	1.0	—		1.0
			S_1	S_2			S_1		S_2			
7	15	15	20	20	15	15	4	2	1.7	1.3	1.0	0.5	0.0

In all cases only a trace of the light key component appears in the bottoms and only a trace of the heavy key component appears in the overhead.

TABLE IB

Comparison of Values of R_m and d_s at R_m

Problem	Underwood Equations d_s	R_m	Colburn Correlation d_s	R_m	Equation 6 d_s	Tray. Calc. d_s	/ R_m
1	10.95	1.24	10.98	1.24	11.2	11.0	1.24
2	12.90	2.085	13.02	2.085	12.5	12.9	2.085
3	13.05	2.28	13.4	2.16	12.5	——	——
4	18.1	1.11	18.1	1.12	18.3	——	——
5	13.30	1.42	13.30	1.42	13.71	——	——
6	11.2	1.40	10.7	1.38	11.2	——	——
	ds_1 ds_2		ds_1 ds_2		ds_1 ds_2		
7	16.81 10.9	2.00	16.8 9.95	1.99	17.0 9.96		

TABLE II

Tray Requirements and Ratio of Key Components on Feed Tray
For Different Distributions of a Split Key

Problem		Mols Feed		d	q	ds Rm at Rm		ds at total Reflux	R	ds	Trays	r_f	Calc. r_f opt.	ref(9) r_f opt.
(1)	lk	30	2.0	28	1.0	1.6	20	24.5	2.0	17.7		—	.85	.94
	s	40	1.5							22.0	19.8	.947		
	hk	30	1.0	2						23.0	19.09	.904		
										24.0	19.00	.855		
										25.0	19.01	.813		
										28.7		—		
(2)	lk	30	2.0	28	1.0	1.6	20	24.5	4.0	12.43		—	.82	.82
	s	40	1.5							20.0	12.0	1.33		
	hk	30	1.0	2						23.0	10.55	1.00		
										25.0	10.2	.724		
										27.0	10.7	.502		
										30.0	12.7	.308		
										33.0		—		
(3)	lk	22.5	2.0	21.0	1.0	1.72	15.38	18.32	4.0	15.4	11.98	1.23	.80	.807
	s	30.0	1.5							18.32	10.5	.80		
	hk	22.5	1.0	1.5						21.0	10.9	.45		
	h	25.0	0.5	—										
(4)	l	25.0	4.0	25.0	1.0	.978	13.48	18.32	4.0	15.0	9.7	1.91	.81	.82
	lk	22.5	2.0	21.0						18.3	8.65	.81		
	s	30.0	1.5							21.0	9.6	.33		
	hk	22.5	1.0	1.5										
(5)	c_1	3.0		3.0	.69	.74	14.04	11.4	1.75	11.4	10.1	.30		
	c_2	7.0		7.0						14.0	10.1	.25		
	c_3	15.0		14.7										
	c_4	33.0												
	c_5	30.0		0.2										
	c_6	12.0												

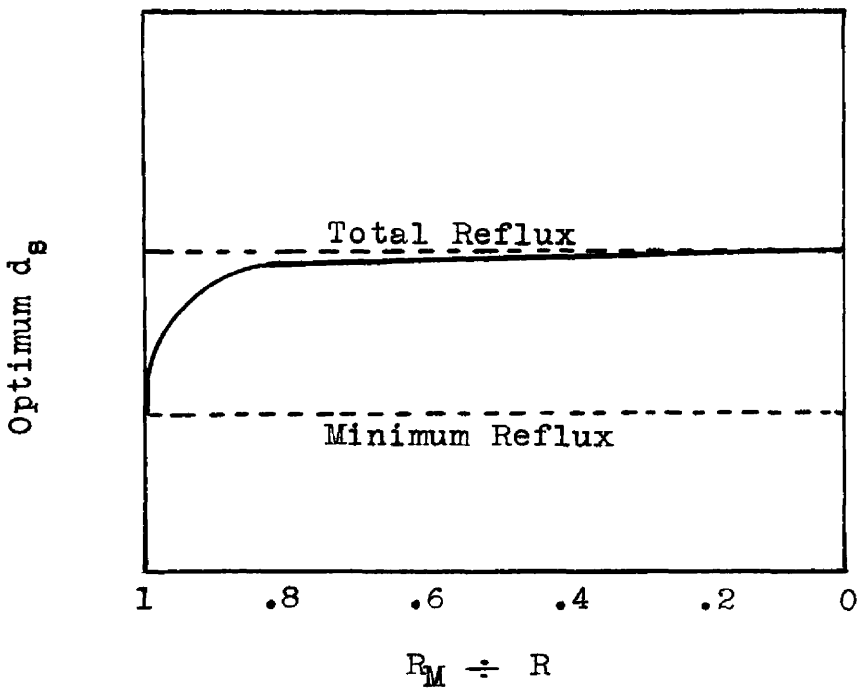

Figure 1 -- Mols of a Split Key Overhead For Minimum Trays.

Discussion:

The results of Table IB for the Colburn correlation were obtained by neglecting the correction factors in the ψ term. In general, this is permissible without appreciable error if the relative volatility of the light components does not approach that of the light key component and the relative volatility of the heavy key components does not approach that of the heavy key component.

In problem (3) if the correction factors in the ψ term had been used the value of $R_M = 2.23$ and $d_s = 13.56$ would have been obtained. Thus, the minimum reflux value has been improved, but the distribution of the split key has become more divergent from the correct value.

A further discrepancy is noted in problem (6). If, with this system, the relative volatility of the light component is varied from ∞ to 2 the distribution of the split key starts at 11.14 (for $\alpha = \infty$), falls to a minimum of 10.94 at $\alpha = 3.0$ and then rises again to 12.5 at $\alpha = 2.0$. This variation may be followed by the equations of Underwood, but if the Colburn correlation is utilized there is a continuous decrease in d_s as α varies from ∞ to α_{lk}.

The above discrepancies are explained by the fact that Colburn's correlation is no longer accurate when the relative volatility of the light or heavy components approach that of the light key or heavy key component, respectively.

However, this is not a serious limitation since it represents an extreme case and in many cases can be overcome. For example, if an isomeric separation such that $\alpha_h \rightarrow \alpha_{hk}$, the mols of the heavy key component overhead may be sufficiently large that the heavy key component may be considered as a split key which lies outside of the relative volatility limits of the specified key components.

In the depropanizer problem, illustrated by both methods of calculation, the serious limitation of the Underwood equations may be illustrated by the fact that there is a 20% deviation between the minimum reflux obtained if the values of α at the fractionating pinch temperature is used and the corresponding value by using α at the temperature of the stripping pinch. By using α_{av} as in the illustration there is 7.5% difference between the value of R_M obtained and that determined by the Colburn correlation. Thus, for cases in which there is appreciable variation of the relative volatilities, the proper feed tray temperature at which to evaluate the relative volatilities for use in the Underwood equations becomes of primary importance. Since the feed tray temperature must lie between the two pinch temperatures, arithmetic average values of α's taken at the pinch temperatures is recommended.

It may be noted that the application of Underwood's equations to split keys is analagous to calculating different pinch compositions using the Colburn correlation. This suggests that the values of relative volatility should be evaluated at different temperatures for

each value of ϕ . Further evidence of this is obtained from the depropaniser problem illustrated. If the same set of average relative volatilities are used by both methods the results are almost precisely identical. However, having obtained R_M and d_s by the Colburn correlations as illustrated, there is no one temperature which permits the checking of R_M and d_s simultaneously when Underwood's equations are used. This check can be obtained only by using different temperatures for the evaluation of each value of ϕ . For example, if the value of ϕ for $\alpha_{LK} > \phi > \alpha_s$ is evaluated at the temperature of the stripping pinch and the value of ϕ for $\alpha_s > \phi > \alpha_{HK}$ is evaluated at the temperature of the fractionating pinch, then $R_M = 0.74$ and $d_s = 14.4$ which is a much better check with the Colburn correlation. No other examples were tried, however, to see if this is a special or general phenomena.

The fact that the distribution of the split key is such that the ratio of the mols of the split key component in the fractionating pinch to that in the stripping pinch lies between the corresponding ratios of the light key component and the heavy key component has been verified by numerous calculations. The assumption that these ratios are precisely linear with respect to $(\alpha - 1)$ has not been verified. However, the assumption of a linear relation represents the average results with good accuracy and permits the use of values in the questions developed which are of a necessity determined in the calculation of the pinch compositions. Further, in most cases a very precise distribution of the split

key is not essential for the determination of a good value of minimum reflux. For example, if the calculated mols of the split key overhead is greater than the true value, the calculated values of L_n and D are both greater than the true values and the ratio, $R_M = L_n/D$, tends to remain constant.

A qualitative representation of the optimum mols of a split key overhead is shown in Fig. 1. It is seen that the optimum mols of the split key component overhead very rapidly approaches the distribution at total reflux as the reflux ratio is increased above the minimum.

It may be noted in the depropanizer problem that the same number of trays was obtained using the distribution for minimum reflux as with the distribution for total reflux. Actually this is not quite correct, but for this problem the distribution of the split key wasn't sufficiently critical to show up in the tray calculations.

Even though Table II isn't very extensive, the conclusions, which have been made on the basis of the results tabulated, can be accepted without appreciable doubt for the following reasons:

1. Since a minimum number of trays is obtained at total reflux, it is not unreasonable to expect the distribution obtained at total reflux to give a minimum number of trays at other reflux ratios.
2. The problems in Table II were selected such that they represent extreme cases; i.e. for most problems encountered

the distribution at minimum reflux and total reflux will agree closer than for the problems given in Table II.

Conclusions:

Either the Colburn correlation or Underwood's equations may be used to obtain the distribution of split keys and minimum reflux. For a poor separation of the key components and constant relative volatility the equations of Underwood are less time consuming. For a sharp separation of the key components and constant relative volatility the time required for calculation is about the same for both methods. For cases in which the relative volatility is not constant the Colburn correlation is more reliable.

The distribution of split keys at total reflux may be obtained by means of the Fenske equation.

For any reflux ratio between the minimum and total the optimum distribution of split keys is very near the value given by the Fenske equation for total reflux.

NOMENCLATURE

c - correction factor
d - mols of a component in the overhead
D - total mols of overhead
K - equilibrium constant
l - mols of a component in the liquid phase
L - total mols of liquid downflow in tower
M - mols of a component (liquid plus vapor)
m - pseudo ratio of liquid to vapor
q - heat required to convert one mole of the feed to saturated vapor divided by the latent heat of the feed
R - mols of reflux per mol of overhead
r - ratio of mols of light key component to heavy key component
S - number of equilibrium steps
V - total mols of vapor upflow in tower
w - mols of a component appearing in the bottoms
X - mol fraction of a component in the liquid phase
Z - total mol fraction of a component (liquid plus vapor)
  - relative volatility of a component with respect to the heavy key component
  - empirical factor defined by equation (11a)
  - defined by equation (1) and has a value between the relative volatilities of the key components.

Subscripts:

av - average
D - overhead
F - feed
f - feed tray
h - heavy component (volatility less than that of the heavy key component)
hK - heavy key component
l - light component (volatility greater than that of the light key component)
L - liquid in feed
lK - light key component
m - stripping section
M - minimum
n - fractionating section
s - split key component
T - top of tower
V - vapor in the feed

Superscripts:

' - denotes uncorrected value

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AUTOBIOGRAPHY

The writer, Raymond Victor Bailey, was born November 23, 1923, in Strong, Arkansas. After the usual grammar and high school education, he entered Louisiana Polytechnic Institute in 1940 and graduated four years later with a Bachelor of Science degree. Immediately after graduation he went to work for Cities Service Refining Corporation at the refinery in Lake Charles, Louisiana, as an analytical chemist. After spending eleven months in the company's employ, he entered the Army of the U. S. A. in January, 1945. After six months in the infantry and twelve months as a chemist with the Sixth Army Regional Laboratory at the Presidio of Monterey, California, he was honorably discharged and entered the Graduate School of Louisiana State University and Agricultural and Mechanical College in September, 1946. In June, 1948, he was awarded the Master of Science degree by the Louisiana State University.

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EXAMINATION AND THESIS REPORT

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Major Field: Chemical Engineering

Title of Thesis: Simplified Multicomponent Fractionation Calculations

Approved:

Jesse Coates
Major Professor and Chairman

W. O. Dowgs
Dean of the Graduate School

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Date of Examination: December 17, 1948